Predicting the environmental fate and ecotoxicological and toxicological effects of pesticide transformation products

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PhD Thesis

University of York
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October 2009

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October 2009

Abstract

Following the application of pesticides during normal agricultural practice these compounds can degrade to form transformation products. When assessing the risks posed by pesticides it is important to include any additional risks posed by these compounds. Current guidance within the EU suggests that data requirements for transformation products during the risk assessment do not necessarily need to be addressed with experimental studies but alternative techniques can be explored and used. Therefore the aim of this research was to investigate and develop pragmatic approaches for assessing the fate and effects of transformation products in the absence of experimentally determined data.

Approaches designed to provide information on the physico-chemical properties, environmental parameters, ecotoxicology and toxicology of pesticide transformation products are explored and evaluated, and recommendations made on how to obtain the most appropriate estimates of these factors. Hydrophobicity, dissociation constant, soil sorption, daphnid aquatic ecotoxicology and rat oral lethality can all be estimated with confidence.

Moreover, approaches were developed to 1) indicate whether a transformation product may exhibit pesticidal activity and subsequently estimate its acute aquatic ecotoxicity in the absence of experimental data, 2) combine well known techniques and experimental data to obtain estimates of transformation product mutagenicity with limited risk of obtaining false negatives and 3) prioritise transformation products of most concern to drinking water supplies and its consumers.

Overall, recommendations are made throughout this thesis on appropriate approaches and methods for generating estimates of transformation product properties, ecotoxicity and toxicity for use in risk assessment and prioritisation frameworks.

Acknowledgements

Studying for this PhD over the past seven years has been a long and eventful journey which has seen a change in University, a change in jobs, moving house twice and gaining a beautiful son, Dillon. Over this period many people have provided guidance and support in both my professional and personal life and it is difficult to name everyone but I would like to say a big thank you to you all, particularly friends at the Cranfield Centre for EcoChemistry and at the EcoChemistry team of the Food and Environment Research Agency.

I would like to thank Dr Alistair Boxall who persuaded me to start this PhD seven years ago and through all that time has provided advice, support and guidance not only during my study but also during my career development.

I would also like to than Ann Ainsley for her help with statistics, Qasim Chaudhry for his help with QSAR and Helen Glover for populating my reference software so thoroughly. I would like to thank John Solbé, Allan Walker, Joop Hermens, Paul Ashby and Mark Clook for comments on earlier versions of Chapter 4. I would like thank the workshop participants and organising committee (Steve Maund, Dana Kolpin, Kathrin Fenner, Andrew Craven and Alice Fulmer) who provided input for the approach proposed in Chapter 5 as well as the comments from Simon Parsons on earlier versions of Chapters 2 and 5. I would also like to thank Miles Thomas for the supply of pesticide estimates of usage. In addition I would like thank all the funding organisations that have made this research possible including Department of Environment, Food and Rural Affairs, Pesticide Safety Directorate and American Water Works Association Research Foundation and its Co-funding Utilities.

Finally this thesis would not have been possible without the support of my family, my deepest felt love, gratitude and thanks go to Elaine, without whose support, friendship and motivation I would never have completed this study.

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Author's Declaration

The work in this thesis was undertaken as a part-time PhD student based initially within the Cranfield Centre for EcoChemistry, Cranfield University at Shardlow (October 2002 – September 2004) and then within the EcoChemistry Team at the Food and Environment Research Agency (formerly the Central Science Laboratory) and the University of York (October 2004 – October 2009).

The research was undertaken whilst performing projects for Government departments (Defra, PSD) and non-governmental organisations (AwwaRF) and have therefore previously been presented to the funding bodies in the form of research reports. Subsequently Chapters 4 and 5 have been written as papers for international peer-reviewed journals. Within this thesis these papers have been reworked to maintain a consistent style and format, however the copyright for these papers rests with the publishers.

Chapter 4 - Sinclair C.J. and Boxall A.B.A. (2003) Assessing the ecotoxicity of pesticide transformation products, Environmental Science and Technology, 37:4617-4625.

Chapter 5 - Sinclair C.J., Boxall A.B.A., Parsons S.A., and Thomas, M.R. (2006) Prioritization of Pesticide Environmental Transformation Products in Drinking Water Supplies, Environmental Science and Technology, 40:7283-7289.

All papers and reports presented in this thesis have joint authorship and reflect the contribution of the main co-author in the role of supervisor (Dr. Alistair Boxall). All were written by the candidate as leading author, however it should be noted that all papers and reports have gained through suggestions and advice from co-authors and the published papers have also benefitited from the comments of anonymous referees as part of the review process.

1 Introduction

1.1 The control of pests

Plant protection products, commonly known as pesticides play an important role in modern intensive agriculture and are used to increase crop quality and yield to meet quantity and quality requirements of consumers. They are employed to control pests or elicit a desired response in the growing crop or final product. Pests fall into many categories but can be considered as any organism having an undesired effect on the output of the agricultural practice. They can compete for resources, bestow disease, directly or as a vector, and/or cause crop damage often through feeding activities.

The application of chemicals to control pests is not a modern concept, the use of sulphur powder dates back thousands of years. Compounds based on organic chemistry and exhibiting modes of action still used in modern pesticides were not identified till the nineteenth century, e.g. the extraction of pyrethrum from the flower heads from *Tanacetum sp* (Tomlin 2006). The development and implementation of modern synthetic pesticides is generally attributed to the middle of the twentieth century triggered by the development of dichlorodiphenyltrichloroethane (DDT) used during World War II for the control of mosquitoes and later employed in agriculture and public health to great effect (Mellanby 1992). DDT went from hero to villain in a relatively short space of time with Paul Müller winning a Nobel Prize in 1948 for identifying the potent effect of DDT on arthropods (Cremlyn 1991), whilst only fifteen years later it was suggested that organochlorine insecticides were drastically effecting bird populations (Carson 1963; Blus et al. 1971). Today, from those humble beginnings we have an impressive array of pesticides exhibiting a multitude of modes of action against a vast range of pests. Together with chemical development, there has also been extensive progress developing the most comprehensive chemical risk assessment process to ensure human and environmental safety.

1.2 Pesticide degradation

Pesticidal persistence in environmental matrices plays a critical role when determining the risk a compound may pose to humans and ecosystems. Following application these organic compounds can be susceptible to abiotic and biotic degradation, e.g. hydrolysis, photolysis or the action of microflora. Microbial populations can become adapted to individual chemicals resulting in increased rates of degradation in soils previously exposed to the compound (Smith and Aubin 1991). During pesticide mineralisation a range of compounds can be formed, which can collectively be termed metabolites, degradation products, degradates and transformation products. In this thesis these compounds will be referred to as transformation products. These compounds can be very similar to the parent molecule due to small changes in structure or can be significantly different due to molecular cleavage forming substantially different compounds.

The pesticide risk assessment process specified in EU Directive 91/414/EEC (European Commission 1994) its subsequent amendments and supporting documents does have provision assessing the risk of transformation products but it is only required for those determined to be relevant. Determining relevance can include measures of, but not limited to, molecular size and composition, amount formed, ecotoxicity and bioaccumulative potential.

During pesticide risk assessments it is common practice during regulatory studies to identify only the transformation products formed in the greatest amounts, e.g. usually $\geq$10% of the applied parent pesticide. However during academic studies that have the ability to explore the capability of more and more competent analytical equipment, many transformation products from just one pesticide can be identified. For example within the UK Pesticide Safety Directorate evaluation document for alachlor, three transformation products were identified in studies examining degradation in natural waters (PSD 1990a), whilst a subsequent academic study identified in excess of twenty transformation

products from alachlor in groundwaters, numerous at relative low levels (Potter and Carpenter 1995).

1.3 Risk of transformation products

Some transformation products have been shown to be more mobile (Brouwer et al. 1990), more persistent (Bromilow et al. 1999), more ecotoxic to non-target organisms (Stratton and Corke 1982; Jones and Winchell 1984) and can be present in surface waters (Thurman et al. 2000; Kalkhoff et al. 2003) and groundwaters (Kolpin et al. 1996b; Kolpin et al. 1997). Therefore it is important that any additional risks posed by these compounds are also considered when determining the risk of parent pesticides (Kolpin et al. 2001). To determine the risk, through experimental studies, for a large number of transformation products from any one pesticide could be a drain on resources. Therefore for that reason guidance has suggested that alternative means could be used, rather than experimentation to provide the required data (European Commission 2002a).

1.4 Aim and objectives

The overall aim of this PhD is to investigate and develop pragmatic approaches for assessing the fate and effects of transformation products in the absence of experimentally determined data. Specific objective are:

1. To identify relationships that exist between parent pesticides and their transformation products in terms of the physico-chemical properties, ecotoxicology and toxicology;
2. To identify and evaluate methods by which the most important physico-chemical properties and effects of transformation products can be estimated;
3. To develop approaches for assessing the ecotoxicity, toxicity and pesticidal activity of transformation products to non-target organisms; and

4. To develop methodologies for identifying and ranking those transformation products that could pose the greatest risk to the public through exposure via drinking water.

1.5 Format of the presentation

The aim and objectives have been addressed in six chapters which constitute this thesis. At the end of this introduction a diagrammatic thesis overview is provided (Figure 1) together with an introduction to the individual chapters below.

Chapter 2 is a review of data from the publicly available scientific literature on the environmental fate of transformation products. Date are collated on the occurrence of transformation products in different environmental compartments, their formation in different systems during the degradation of the parent pesticide together with their mobility and persistence once formed in the environment.

Chapter 3 presents an investigation into transformation products inherent physico-chemical properties and environmental parameters to identify what relationships exist between these and the properties of their parent pesticides. Estimation techniques such as QSAR (Quantitative structure-activity relationships) are also explored to determine whether such approaches are suitable to estimate properties that can be important during the risk assessment process.

Chapter 4 investigates the ecotoxicological impact transformation products may have on non-target aquatic organisms. Explanations for increases in ecotoxicity from pesticides to transformation products are suggested and then used to develop a pragmatic approach for providing a conservative estimate of non-target aquatic acute ecotoxicity in the absence of experimental data. Moreover a qualitative approach for identifying whether a transformation product may

exhibit the specific mode of action of the parent pesticide based on the identification of structural moieties is proposed.

Chapter 5 contains the development of a risk based prioritisation approach that can be applied to different geographical regions to identify which pesticide metabolites should be of most concern in terms of their potential to contaminate source drinking waters and subsequently pose a risk to consumers.

Chapter 6 investigates the mammalian toxicity of transformation products, specifically mutagenicity and rat oral LD50. Attempts are made to identify the general relationships between pesticide and transformation product toxicity and whether predictive approaches are suitable methodologies for their estimation.

Chapter 7 is the final chapter that attempts to bring this research together, evaluates some of the proposed methodology against recently released approaches, discusses some of the most important issues concerning pesticide transformation products in the environment and provides suggestions on what further research is required for pesticide transformation products.

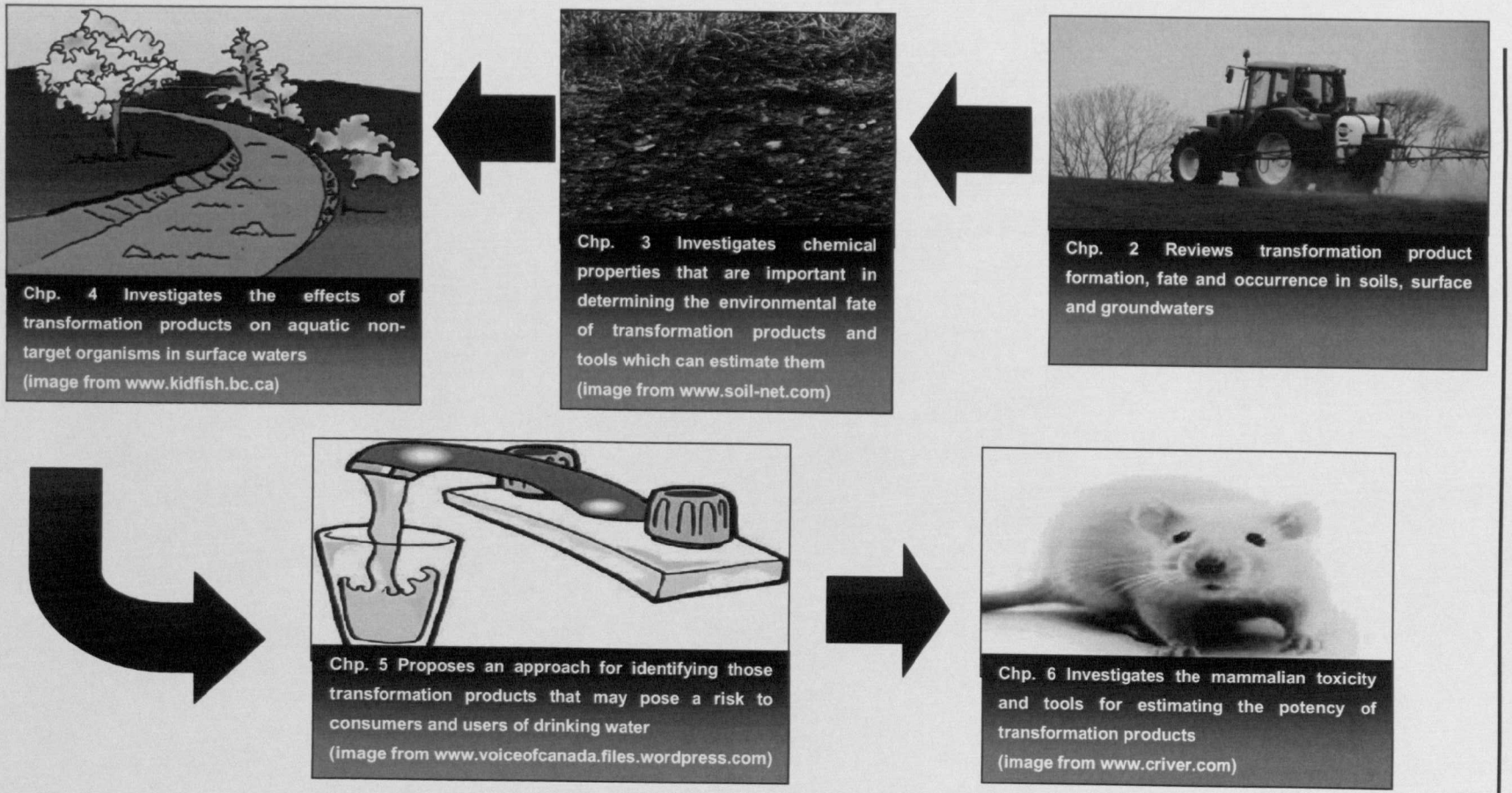

Figure 1. Diagrammatic representation of this thesis

2 Transformation Products in the Environment

2.1 Introduction

Once released into the environment, pesticides are susceptible to degradation by biotic and abiotic means. This can result in the formation of a range of compounds (Roberts 1998; Roberts and Hutson 1999). The transformation of a pesticide includes all processes where structural change takes place (Somasundaran and Coats 1991). Therefore, pesticide transformation can produce a diverse range of compounds and it is important that transformation products are considered when determining the risks to the environment and human health posed by their application. However, the risks posed by transformation products should not be considered individually but always in conjunction with the risks posed by parental pesticides.

Once pesticides are applied during agricultural practice there is the potential for transformation products to form. These compounds together with the parent pesticide can then, depending on properties, move from the soil to other environmental compartments. Some compounds can volatilize into the air and move large distances in the particulate or gaseous phase and be deposited by rainfall large distances away from the site of application (Goolsby et al. 1997; Majewski et al. 1998). Some can move vertically through the soil profile to groundwater and then away from the site of application via aquifer transport (Schiavon 1988; Widmer and Spalding 1995; Broholm et al. 2001). Additionally, there is also the potential for these compounds to enter surface waters when they travel laterally either via overland runoff due to heavy rainfall or via sub-soil tile drains, entering agricultural ditches and streams and then on to major rivers, reservoirs and ultimately to estuaries and the marine environment (Muir and Baker 1976; Phillips et al. 1999; Aga and Thurman 2001).

With pesticide transformation products entering major rivers, reservoirs, and groundwater, there is the potential for these compounds to be present in water abstracted for drinking water treatment (Heberer and Dünnbier 1999). Whether these transformation products are present in this raw water will depend on their rate of formation in the environment, the extent of their parental use in the particular catchment, and the physico-chemical properties and rate of degradation of themselves and their parents (Boxall et al. 2004). When considering the movement of transformation products through the environment, the movement of the parent pesticide needs also to be considered, because any point along the pesticide 'journey' can witness degradation and the formation of additional transformation products. Therefore, transformation products with low mobility can occur a distance from the site of application (Brouwer et al. 1990).

Drinking water standards specific to particular transformation products are limited in the USA (aldicarb sulfone and sulfoxide), whilst in the EU transformation product drinking water standards are covered by the 0.5μg L^{-1} limit for total pesticides (and their 'relevant metabolites'). The term 'relevant metabolite' was introduced in the EU Directive 91/414/EEC (European Commission 1994) and its subsequent amendments. This legislation concerns the placing of plant protection products on the market and subsequent guidance has been provided on determining the relevance of a transformation product (European Commission 2003). Water treatment processes designed to remove pesticides may not be as efficient at removing the smaller, more polar transformation products. An important consideration during drinking water treatment is the additional formation of transformation products from either the pesticides or the environmental transformation products (Zhang and Pehkonen 1999).

Available information relating to the monitoring and measurement of transformation products in the environment is dominated by the triazine and chloroacetamide herbicides (e.g. Thurman et al. 1991; Pereira et al. 1992; Albanis and Hela 1998; Boyd 2000). A large volume of data are available

concerning the environmental occurrence of the cotton and corn herbicides from studies performed in the USA. Their environmental fate and that of their transformation products has been documented for soil, sediment, surface waters including runoff, streams, rivers, estuaries, lakes and reservoirs, ground waters, rain and air (e.g. Muir and Baker 1976; Assaf and Turco 1994; Lerch et al. 1995; Thurman and Cromwell 2000; Scribner et al. 2000). A large proportion of the available work focuses on atrazine, while cyanazine, metolachlor, and alachlor are also studied in detail. The main transformation products under investigation were: deethylatrazine (DEA), hydroxyatrazine (HA) and deisopropylatrazine (DIA), cyanazine amide and the ethane sulfonic acids (ESA) and oxanilic acids (OA) of metolachlor and alachlor.

In this Chapter, information from the literature and industry data are used to identify the nature and amounts of pesticide transformation products that are formed in the environment through biotic degradation, e.g. soil and sediment or abiotic degradation pathways, e.g. surface and aqueous photolysis or hydrolysis. Information is also presented on their occurrence, persistence and mobility in the environment.

2.2 Formation in the Environment

Once pesticides are applied in the environment during either normal agricultural practice or via alternative uses such as domestic, industrial, and amenity, they are susceptible to biotic and abiotic degradation. The major abiotic processes include hydrolysis, photolysis, and oxidation/reduction. Hydrolysis is a chemical transformation process in which an organic molecule reacts with water. Substances that are potentially susceptible to hydrolysis include alkyl halides, amides, amines, carbamates, epoxides, nitriles, phosphoric acid esters, and sulphonic acid esters (Samiullah 1990). Photolytic degradation can occur directly (where the substance itself absorbs solar radiation) or indirectly (where the energy is transferred from some other species).

Biodegradation is one of the most important forms of degradation in the environment (Pavel et al. 1999; Rice et al. 2002). It is generally a significant loss mechanism in soils and aquatic systems and is essential to wastewater treatment. Although higher organisms can metabolise a substance, it is the microbes that play the most important role in the degradation of a substance in environmental media. The majority of biodegradation reactions can be categorized as oxidative, reductive, or conjugative (Hill 1978) (Table 1).

Table 1. Examples of biodegradation reactions that are relevant to pesticides (Hill 1978)

Type of reaction	Example(s)
ß-oxidation	Phenoxyalkanoates
Oxidative dealkylation; N-dealhylation	Alkyl carbamates, phenylureas, s-traizines
O-dealkylation	Organophosphorous pesticides, phenoxyalkanoates
C-dealkylation	Methoxychlor
Thioether oxidation	Carbophenothio, prometryn, aldicarb
Decarboxylation	Nicotinic acid
Epoxidation	Aldrin, heptachlor
Aromatic hydroxylation	2,4-D, nicotinic acid
Aromatic, non-heterocyclic ring cleavage	Catechols, phenols, phenoxyalkanoate herbicides, carbaryl
Aromatic, heterocyclic ring cleavage	Paraquat, picloram, amitrole
Hydrolysis	Carbamates, organophosphates, urea and anilines
Hydrolytic dehalogenation	TCA, dalapon, chlorobenzoates
Halogen migration	Anisoles, 2,4-D
Reductive dehalogenation	DDT
Dehydrohalogenation	p,p-DDT, lindane
Nitro-reduction	Parathion

Selected transformation products identified in the environment can result from multiple pesticides or even from non-pesticidal sources. For example, the transformation product DIA is a transformation product of three triazine herbicides: atrazine, cyanazine, and simazine; while DEA is a transformation product of atrazine, propazine, and cyprazine (Muir and Baker 1976; Thurman et al. 1994; Scribner et al. 2000) (Figure 2). The chlorinated phenols, e.g. 2,4-dichlorophenol, a transformation product of the herbicide 2,4-D, can enter the environment either during their manufacture and use or via the degradation of phenoxycarboxylic acids. Therefore, when monitoring the occurrence of transformation products in raw water sources such as rivers and groundwater, in some cases it may be difficult to identify the particular source of a transformation product.

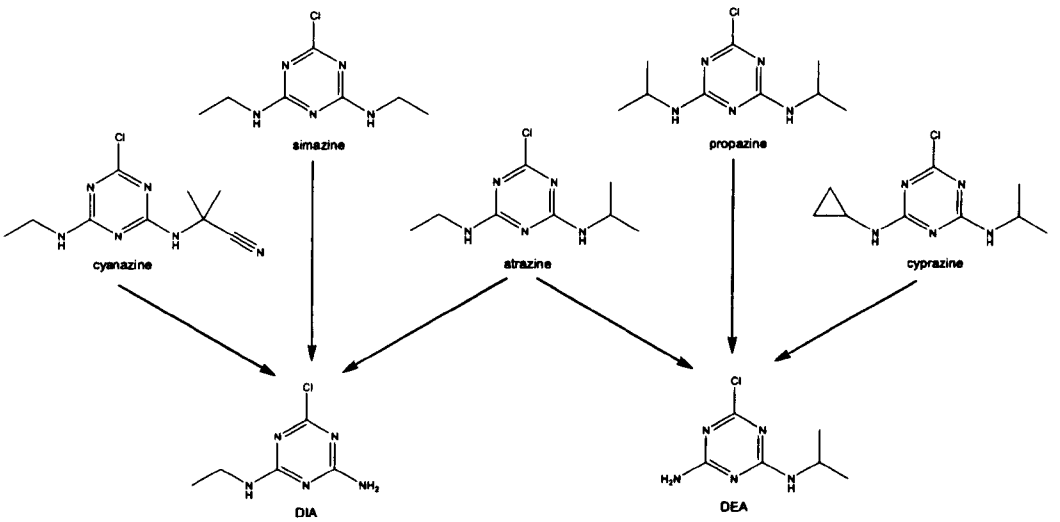

Figure 2. Degradation of the triazine herbicides to deisopropylatrazine and deethylatrazine (adapted from Scribner et al. 2000)

The structural changes seen between a pesticide and transformation product can be large or small alterations of a single structural moiety. Structural cleavage generally forms two much smaller compounds such as the hydrolytic cleavage of the sulfonylurea herbicides. The process of pesticide degradation does not have to be a reduction in structural size. Transformations can also slightly alter the structure of a pesticide, producing a structurally similar transformation product such as the hydrolytic de-chloroination of the chloroacetamide herbicides (Roberts 1998) (Figure 3).

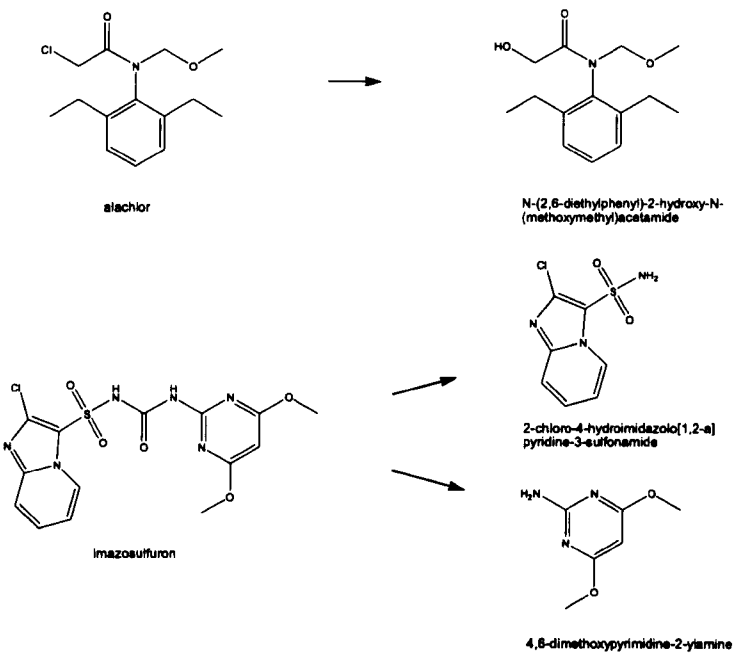

Figure 3. The transformation and cleavage degradation pathways of chloroacetamide and sulfonylurea herbicides

When a small modification to a pesticide's structure occurs and the majority of the pesticide structure is still intact, it is possible for the transformation product to maintain the same specific mode of action of the parent compound. Some pesticides are specifically designed to use a process such as this to enable greater efficiency. The precursor compound can be more stable or can enter the target organism more effectively. A transformation then takes place, producing the more active pesticide. Pesticides that act in this manner are known as pro-pesticides which includes the thiophosphate class of organophosphorus insecticides which undergo oxidative desulphurisation once in the target organism to the oxon form, which are much more potent acetylcholinesterase inhibitors (Drabek and Neumann 1985) (Figure 4). In the environment, the transformation of the pro-pesticide to the active form can occur. Current legislation in Europe for placing new pesticides on the market ensures that the environmental risk assessment process considers the active component of a pesticidal application (European Commission 1994).

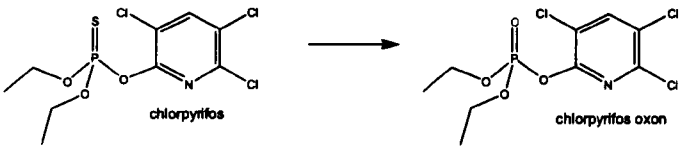

Figure 4. The oxidative desulphurisation of the insecticide chlorpyrifos

When pesticides are released into the environment a number of different transformation products can be produced. The extent of pesticide degradation and the identity and quantity of transformation products formed depend on the degradation pathways and environmental conditions that are experienced (Roberts 1998; Roberts and Hutson 1999). Transformation product formation in soil is influenced by soil properties and conditions, these can be inherent properties such as soil texture or transient properties such as organic carbon content, microbial ecology, water content and pH.

The structural identity of transformation products formed during pesticide degradation is not necessarily dependent on the degradation pathway followed, e.g. during the aerobic and anaerobic soil degradation of carbaryl, 1-napthol is formed from both pathways, while 2-hydroxy-1,4-napthaquinone is only formed via aqueous photolysis (Figure 5). Due to the high total usage of pesticides in agriculture when compared to other applications (Donaldson et al. 2002), pesticide degradation in soil is one of the most important processes determining which transformation products could be present in other environmental compartments. Many factors determine the rate and route of pesticide degradation and hence, transformation product formation. Once a pesticide has undergone a degradation step, additional transformation products can then be formed from this transformation product and alternative transformation products formed from the pesticide via a different degradation pathway. Following application of triazine herbicide atrazine, transformation product concentrations in the vadose zone were in the order DEA > didealkylatrazine > DIA > hydroxyatrazine (HA). In the following season when atrazine was not applied,

transformation product concentrations were in the order didealkylatrazine > DEA > DIA > HA. This change in transformation product concentration ratio is due to the degradation of the DEA and DIA to didealkylatrazine (Pashin et al. 2000). This branching degradation of pesticides, influenced by environmental conditions, can therefore produce a wide range of transformation products.

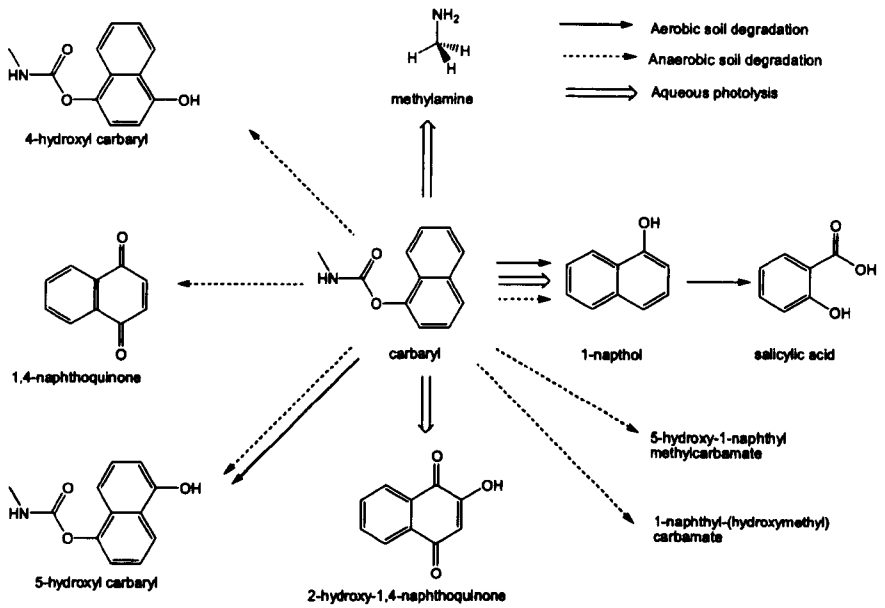

Figure 5. Selected degradation pathways for the insecticide carbaryl (Boxall et al. 2004)

The diversity of the microbial community is very important in the biotic degradation of pesticides. The biotic degradation rate constant of endosulfan is influenced by the degrading microbes; the fungal species *Fusarium ventricosum* can degrade endosulfan faster than the bacterium *Pandoraea sp.* (Siddique et al. 2003). Moreover, microbial communities can adapt to degrade compounds, increasing the degradation rate constant of a compound following its subsequent application and therefore, transformation product formation (Smith and Aubin 1991). However, not all pesticides show this increase in degradation rate constants following repeated application as some compounds show no change, e.g. chlorpyrifos, while others show a reduction in degradation rate constants, e.g. chlorothalonil (Singh et al. 2002). Generally, the biotic degradation of

compounds decreases with depth through the soil profile, due to the decrease in microbial biomass and organic carbon content. The degradation of the chlorpyrifos primary transformation product, 3,5,6-trichloro-2-pyridinol, adheres to this principle whilst the degradation rate constants of the parent compound can increase down the soil profile. This increase in the chlorpyrifos degradation rate constant has been attributed to an increase in soil pH with depth in the specific soil (Baskaran et al. 2003). Where soil is amended with organic material such as manure, slurry or straw, pesticide and transformation product degradation rate constants in the top soil can be increased due to the increase in biological activity (Benoit and Barriuso 1997; Wagner and Zablotowicz 1997).

The oxygen levels under which degradation occurs can drastically alter the degradation of pesticides and the formation of transformation products. The degradation rate constants and pathways of a pesticide in soil, sediment or groundwater can vary depending on whether the environmental compartment is under aerobic or anaerobic conditions. The degradation rate constant of alachlor and the formation ratio of two transformation products (alachlor ESA and alachlor OA) differ when under aerobic and anaerobic conditions (Graham et al. 2000). These two transformation products are commonly identified in aerobic environmental compartments (Kalkhoff et al. 1998; Aga and Thurman 2001). Different transformation products, e.g. acetyl alachlor and diethyl aniline, are identified under methanogenic and sulphate-reducing conditions (Novak et al. 1997).

2.3 Methods for Determining Transformation Routes

A number of approaches are available for identifying transformation products of a pesticide including experimental methods and predictive approaches.

2.3.1 Experimental methods

The pathway of degradation of a substance in soil is typically determined according to specified guidelines, e.g. Organisation for Economic Co-operation and Development (OECD) guideline No. 307 (OECD 2002). Soil is treated with the radio-labeled test substance and incubated in the dark in biometer-type flasks or in a flow-through system under controlled laboratory conditions (at constant temperature and soil moisture). The soil used is typically a sandy loam, silty loam, loam or loamy sand with a pH of 5.5-8.0, an organic carbon content of 0.5-2.5% and a microbial biomass of at least 1% of the total organic carbon. After appropriate interval times, soil samples are extracted and analyzed for the parent compound and transformation products. Volatile products are also collected for analysis using appropriate adsorption devices. The studies are typically performed for up to 120 days. Following removal from the test system, the substrate is extracted and total radioactivity in the extracts is determined by liquid scintillation counting (LSC). Extracts can be further investigated using thin layer chromatography (TLC) and radioscanning, by high performance liquid chromatography (HPLC) with a radiomatic flow detector, or by fraction collection with LSC. Transformation products can be identified by liquid chromatography-mass spectrometry (LC-MS), gas chromatography-mass spectrometry (GC-MS) and nuclear magnetic resonance (NMR).

Sediment/water degradation studies are carried out using a similar approach to the soil degradation studies. Experiments are typically performed on sediments with high and low organic matter contents and are carried out in static systems. The water/sediment systems are pre-incubated to establish an anaerobic environment. During pre-incubation pH, oxygen content and redox potential are carefully monitored. Radio-labeled test substance is added to the water phase and incubated for up to 14 weeks. Carbon dioxide evolution is monitored at regular intervals and both sediment and water phases are analyzed separately for parent compound, major transformation products and bound residues.

2.3.2 Predictive approaches

Degradation route studies are complex and costly, and it is often very difficult to identify the minor transformation products in a system. Information is available for a wide range of pesticides (e.g. Roberts 1998; Roberts and Hutson 1999), but limited information is available for other substances. An alternative to experimental testing might be to use structure-biodegradability relationships (SBR) to predict degradation pathways from the chemical structure of the parent compound. Predictive techniques that estimate toxicity, physico-chemical properties and biodegradation are collectively known as QSAR. A number of systems have been developed for predicting degradation pathways, these include BESS (Punch et al. 1997), PPS (Hou et al. 2003) and CATABOL (Jaworska et al. 2002). BESS is a computerized system that simulates the biodegradation of compounds through sequential application of plausible biochemical reactions (Punch et al. 1997). PSS is a web-based system that can predict biodegradation of most aliphatic and aromatic organic functional groups containing C, H, N, O and halogens (Hou et al. 2003). CATABOL is a probabilistic approach to modeling biodegradation based on aerobic microbial transformation pathways generated from inherent biodegradability tests (e.g. OECD 1981) and expert judgment (Jaworska et al. 2002). CATABOL has been evaluated for determining transformation pathways for pesticides in soil (Sinclair et al. 2003). Comparison of predictions with experimental observations indicated that only 24% of experimentally derived transformation products are predicted correctly. Further development of CATABOL and other expert systems is therefore required before they can usefully be used to identify or predict transformation products.

2.4 Characteristics of Transformation Products of Major Pesticides

Data collated throughout this research on the formation of transformation products in different environmental systems, including aqueous photolysis,

hydrolysis, aerobic soil (laboratory and field), anaerobic soil and sediment/water systems are provided in Appendix A, Table A1. (During 2004 the collated transformation product formation data were investigated, at that point data were available for 215 transformation products formed from 62 pesticides, the discussion below focuses on the data available at that time). 122 transformation products were identified as being formed at ≥ 10% of the applied pesticide in one or more degradation studies. Therefore, based on the definition in the EU, these compounds can be considered 'major metabolites'.

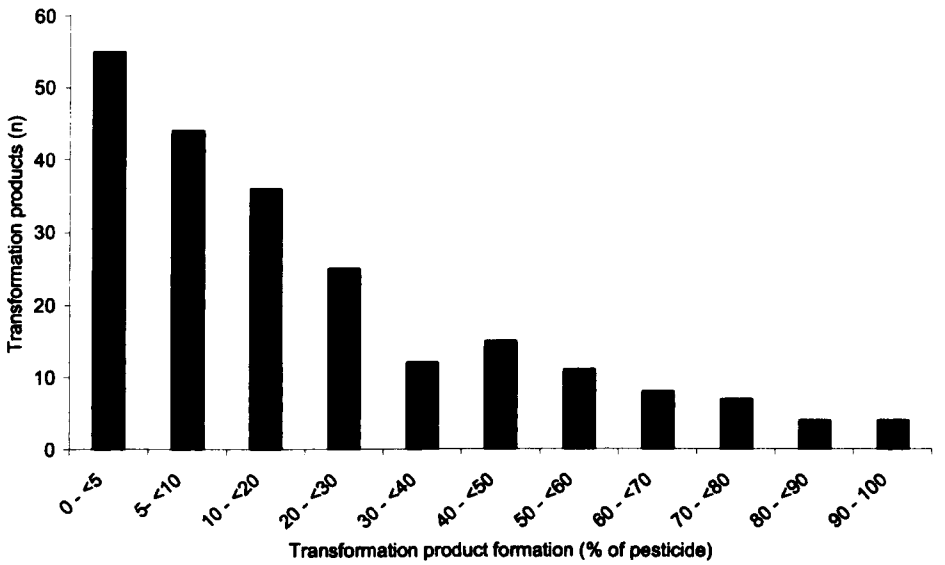

Figure 6. Formation of pesticide transformation products as a percentage of the parent pesticide (each transformation product is represented by the degradation study where it was most prevalent)

The extent of transformation product formation is presented in Figure 6, where each identified transformation product is represented by the extent of its formation in the degradation study where it was most prevalent. There are a number of transformation products (8) with a formation >80% of the applied pesticide. Four of these compounds are pesticides that act as a pro-pesticide and their transformation to the active component can be expected at a high rate, e.g. diclofop-methyl, fluzifop-p-butyl, fluoroglucofen-ethyl and carbofuran. The

remainder were dihydroxy anilazine from anilazine, ethyl-m-hydroxyphenyl carbamate from desmedipham, propargyl butyl carbamate from IPBC and saccahrin from metsulfuron-methyl. The data in Figure 6 includes aerobic and anaerobic soil degradation, sterile hydrolysis, aquatic and soil photolysis, column and lysimeter leachate studies and degradation in water/sediment systems. The most common formation data available in the literature is transformation product formation during pesticide degradation in aerobic soil; ~44% of data points were of this type.

No conclusions should be drawn about the ratio of major to minor transformation products identified. Degradation studies and the relevant legislation are biased toward identifying those transformation products formed in greater amounts. Due to constraints on time and money, limitations in analytical capabilities, and the perceived unimportance of transformation products formed in small quantities, these compounds are rarely identified or quantified during degradation studies undertaken for the purposes of pesticide registration. For example, when the fate of alachlor is investigated, alachlor ESA, alachlor OA, and 2,6-diethylaniline are commonly identified in surface water, groundwater, soil and sediment (e.g. Graham et al. 1999; Scribner et al. 2000; Graham et al. 2000; Fava et al. 2000; Osano et al. 2003). However, an extensive investigation into the occurrence of alachlor transformation products in groundwater following agricultural application identified at least twenty different transformation products, a number of which occurred in the ng L^{-1} range (Potter and Carpenter 1995). Therefore, a number of transformation products may be formed in quantities two or three orders of magnitude less than the major transformation products of a pesticide. However, the importance of these compounds is probably negligible in most cases when compared to the possible risks posed by either the pesticide itself or its major transformation product(s). A summary of the most prevalent major transformation products formed during aerobic soil degradation studies are provided in Table 2.

Table 2. Summary of the most prevalent major transformation products formed from each pesticide with available data from aerobic soil degradation studies

Transformation product	Parent pesticide [a]	% of pesticide [b]	Time [c]	Reference
(EZ)-3-chloroacrylic acid	1,3-dichloropropene	37%	28 days	EFSA 2006a
2,4-dichlorophenol	2,4-D	11%	-	Roberts 1998
2,4-D	2,4-DB	26.1%	48 days	EU 2002a
methamidophos	acephate	major [d]	-	EPA 2001c
N-(2-ethyl-6-methylphenyl)-2-sulfoneacetamide	acetochlor	> 10%	-	Roberts 1998
2,6-diethyl-N-methoxymethyl-2-sulpho-acetanilide	alachlor	15 - 25%	4 - 7 weeks	PSD 1990a
aldicarb sulfoxide	aldicarb	67 -92%	-	APVMA 2001
HOE 101630	amidosulfuron	49.6%	7 days	PSD 1994a
BTS 27919	amitraz	35%	-	EPA 1996a
dihydroxy anilazine	anilazine	43%	366 days	PSD 1994b
hydroxyatrazine	atrazine	19%	95 days	Assaf and Turco 1994
azoxystrobin acid	azoxystrobin	20%	-	Roberts and Hutson 1999
benalaxyl M2	benalaxyl	34.1%	98 days	EU 2004c
carbofuran	benfuracarb	73 - 93%	0 days	PSD 1998a
bensulide oxon	bensulide	13.8%	270 days	PMRA 2003c
bitertanol benzoic acid	bitertanol	19%	30 days	Roberts and Hutson 1999
M510F49	boscalid	14% [b]	-	PMRA 2004c
3,5-dibromo-4-hydroxybenzoic acid	bromoxynil	16.1 - 34.8% [b]	1 day	EU 2004d
bromoxynil	bromoxynil octanoate	44.6% [b]	4 days	EU 2004d
tetrahydrophthalamide	captan	66%	7 days	EPA 1999a
1-napthol	carbaryl	major [d]	-	EPA 2004d
2-chlorobenzoic acid	clofentazine	major [d]	-	Tomlin 2000
5-amino-4-chloropyridazin-3(2H)-one	chloridazon	43.2 - 46.6%	187 days	Roberts 1998
4-hydroxy-2,5,6-trichloroisophthalonitrile	chlorothalonil	32%	60 days	EPA 1999b
3,5,6-trichloro-2-pyridinol	chlorpyrifos	30 - 38%	14 - 360 days	EU 2005d
3,5,6-trichloro-2-pyridinol	chlorpyrifos-methyl	43% [d]	7 days	EU 2005e
2-chlorobenzene sulfonamide	chlorsulfuron	50%	2 months	PSD 1991a
3-(3-chloro-p-tolyl)-1-methylurea	chlorotoluron	30%	16 - 84 days	EU 2005c
5-chloro-3-fluoro-2-hydroxy-pyridine	clodinafop-propargyl	9 -14%	-	PSD 1995a
cloquintocet acid	cloquintocet-mexyl	<20%	-	PSD 1995a
cyanazine acid	cyanazine	>50%	40 days	Blumhorst and Weber 1992
CCIM	cyazofamid	18.4 - 31.3%	3 -10 days	EU 2002c
T2SO	cycloxydim	48%	7 days	PSD 1990b
compound XV	*lambda*-cyhalothrin	12% [b]	63 days	EU 2001c
4-fluoro-3-phenoxybenzoic acid	cyfluthrin	31% [b]	118 days	EU 2002b
3-phenoxybenzoic acid	cypermethrin	23-48%	364 days	EU 2004b
CGA 249287	cyprodinil	12%	50 days	PSD 1997a
melamine	cyromazine	20 - 44%	29 weeks	PSD 1993a
methylisothiocyanate	dazomet	major [d]	-	APVMA 1997b
decamethrinic acid	deltamethrin	23% [b]	14 days	EU 2002e
ethyl-m-hydroxyphenyl carbamate	desmedipham	16%	7 days	PSD 1993b
pyrimidinol	diazinon	72.9%	14 days	PSD 1991b
3,6-dichlorosalicylic acid	dicamba	31%	6 weeks	Smith 1974
dimethylaminosulfanilide	dichlofluanid	major	-	HSE 2003
2,6-dichlorobenzamide	diclobenil	13.1% [b]	50 weeks	EPA 1998d
2,4-dichlorophenol	dichlorprop	10%	8 days	Haberhauer et al. 1999
diclofop acid	diclofop-methyl	90%	2 days	PSD 1991c
N,N-dimethylacetoacetamide	dicrotophos	20%	5 days	EPA 2002b
4-chlorophenyl urea	diflubenzuron	37% [b]	7 - 14 days	EPA 1997
M9	diflufenzopyr	major	-	PMRA 1999b

Table 2. Summary of the most prevalent major transformation products formed from each pesticide with available data from aerobic soil degradation studies

Transformation product	Parent pesticide [a]	% of pesticide [b]	Time [c]	Reference
N-demethyldimefuron	dimefuron	16.6 - 29.98%	93 days	PSD 1993c
disulfoton sulfone	disulfoton	35%	-	EPA 2002a
N'-(3,4-dichlorophenyl)-N-methylurea	diuron	20.9 - 22.5%	365 days	EPA 2003c
endosulfan sulphate	endosulfan	major [d]	-	EPA 2002c
$CONH_2$-fen	esfenvalerate	32% [b]	12 months	PSD 1992b
triazine amine C	ethametsulfuron-methyl	major	-	PMRA 1992
2-hydroxy ethyl phosphonic acid	ethephon	63.5%	30 days	EPA 1995a
RH-9129	fenbuconazole	major	-	PMRA 2003f
HOE 72829	fenchlorazole-ethyl	36%	2 days	PSD 1990d
3-methyl-4-nitrophenol	fenitrothion	30%	1 - 2 weeks	APVMA 1999
3-phenoxybenzoic acid	fenpropathrin	14%	-	PSD 1989
M3	fenpyroximate	2.6 - 10.8%	14 - 28 days	PSD 1995b
RPA 200766	fipronil	57%	157 days	PSD 2004a
flamprop-M acid	flamprop-M-isopropyl	major [d]	-	Roberts 1998
5-hydroxy-XDE-570	florasulam	72%	3 days	PMRA 2001b
fluzaifop acid	fluazifop-P-butyl	97%	2 days	PSD 1988d
compound XII	fluazinam	11.4%	30 days	PSD 1994d
MKH 6562 sulfonamide	flubcarbazone-sodium	46 - 69%	-	PMRA 2000b
FOE sulfonic acid	flufenacet	14 - 23%	120 days	PMRA 2000c
4-(2-chloro-α,α,α-trifluoro-p-tolyloxy)-2-fluorophenyl urea	flufenoxuron	9.5 - 14% [b]	30 days	HSE 1995
RH-5781	fluoroglycofen-ethyl	79%	21 days	PSD 1992c
FBC 96912	fluquinconazole	28.7%	365 days	PSD 1999b
4-amino-3,5-dichloro-6-fluoromethoxypyridine	fluroxypyr	17.8% [b]	28 days	EU 1999
RE 54488	flurtamone	10.8%	-	PSD 2000a
fomesafen amine	fomesafen	20.5%	59 days	PSD 1995c
carbamoylphosphonic acid	foseamine-ammonium	94%	0 days	EPA 1995c
3-methyl phosphinico-proprionic acid	glufosinate ammonium	52%	95 days	PSD 1990e
aminomethylphosphonic acid	glyphosate	26 - 29% [b]	14 days	EU 2002i
aminomethylphosphonic acid	glyphosate trimesium	15.4% [b]	14 days	EU 2002i
1,2,4-triazole	hexaconazole	> 10%	-	PMRA 1995; PMRA 1999a
3-hydroxy-cyclohexyl-6-(dimethylamino)-1-methyl-1,3,5-triazine-2,4(1H,-3H)-dione	hexazinone	18.7%	365 days	EPA 1994a
1,5-bis(-p-tolyl)-1,4-pentadiene-3-one	hydramethylnon	25.9%	3 months	PSD 1994e
1-(2,4-dichlorophenyl)-2-imidazolylethan-1-ol	imazalil	major [d]	-	Roberts 1998
3,5-di-iodo-4-hydroxybenzoic acid	ioxynil	20.4% [b]	3 days	EU 2004e
ioxynil	ioxynil octanoate	52.6% [b]	-	EU 2004e
propargyl butyl carbamate	IPBC	>90%	6 hours	HSE 1994
RP 30228	iprodione	31% [b]	-	EU 2002j
CA 30-0155	irgarol 1051	>10%	-	HSE 2002
desmethylisoproturon	isoproturon	15.6%	4 weeks	PSD 1995d
2,6-dimethoxybenzoic acid	isoxaben	14%	118 days	Roberts 1998
RPA 202248	isoxaflutole	83 - 68.4%	-	PMRA 2000d
kresoxim-methyl acid	kresoxim-methyl	84%	-	PSD 1997b
malathion dicarboxylic acid	malathion	62%	7 days	PSD 1995e
ethyleneurea	maneb	36.1 - 63.8%	-	EU 2005g
MCPA	MCPA-thioethyl	66% [b]	2 days	EU 2005h
HOE 094270	mefenpyr-diethyl	72.2%	64 days	PSD 1999a
CGA-62826	metalaxyl	53.6%	66 days	EPA 1994b
methylisothiocyanate	metam-sodium	75%	-	APVMA 1997b
amino-N-benzothiazol-2-yl-N-methylamide	methabenzthiazuron	major [d]	-	Roberts 1998
methiocarb sulfoxide	methiocarb	30% [b]	29 days	PSD 1998b
ethylenebisisothiocyanide sulfide	metiram	57% [b]	0 days	EU 2005j
metolachlor oxanilic acid	metolachlor	28.09%	90 days	EPA 1995d

Table 2. Summary of the most prevalent major transformation products formed from each pesticide with available data from aerobic soil degradation studies

Transformation product	Parent pesticide [a]	% of pesticide [b]	Time [c]	Reference
IN-A4098	metsulfuron-methyl	33% [b]	12 weeks	EU 2000a
1,2,4-triazole	myclobutanil	major [d]	-	PMRA 1993
ASDM	nicosulfuron	85.2% [d]	148 days	PSD 2000b
desmethyl norflurazon	norflurazon	31 - 36%	365 days	EPA 1996b
ketone metabolite	paclobutrazol	18% [b]	-	PSD 1995f
MHPC	phenmedipham	54% [b]	5 days	EU 2004f
CL 153815	picolinafen	major [d]	-	PMRA 2003h
dichlorobenzoic acid	piperalin	21%	14 days	EPA 1994c
5,6-dimethyl-2-dimethylamino-pyrimidin-4-ol	pirimicarb	30 - 36%	-	PSD 1994f
2-diethylamino-6-methylpyrimidin-4-ol	pirimiphos-methyl	72 - 75%	-	PSD 1997c
CGA-171683	primisulfuron methyl	88.6%	-	PMRA 2001a
2,4-bis(isopropylamino)-6-hydroxy-s-triazine	prometryn	26.2%	360 days	EPA 1996c
RH24644	pronamide	27%	-	EPA 1994d
propachlor oxanilic acid	propachlor	33.3%	1 month	EPA 1998e
Ro 17-3102	propaquizafop	25.9 - 38.8%	1 month	PSD 1994g
CGA 118 245	propiconazole	22%	-	EU 2003e
propylene urea	propineb	40% [b]	2 days	EU 2003f
N-(1,1-dimethylacetonyl)-3,5-dichlorobenzamide	propyzamide	77%	-	Roberts 1998
CGA 180777	pymetrozine	16.5%	-	PMRA 2002
6-chloro-3-phenyl-pyridazin-4-ol	pyridate	88% [b]	3 days	EU 2001d
ZK 512723	pyrimethanil	52 - 58%	186 - 243 days	PSD 1995g
BH518-2	quinmerac	42.4%	224 days	PSD 1998c
quizalofop acid	quizalofop-methyl	36%	15 days	PSD 1987
IN-70941	rimsulfuron	30.3 - 33.1%	365 days	PSD 1996
hydroxysimazine	simazine	<0.1 - 11%	294 days	PSD 1992d
sulphonamide	sulfosulfuron	12.8% [b]	-	PMRA 1998
haloaniline	tau-fluvalinate	10% [b]	-	PSD 1997d
3,5-dichloro-2,4-difluorophenyl urea	tebflubenzuron	10.4%	-	PSD 1991d
2,3,5,6-tetrafluoro-4-methylbenzoic acid	tefluthrin	10% [b]	122 days	PSD 1991e
tetraconazole acid	tetraconazole	~80%	7 days	PSD 1999c
thiophene sulfonimide	thifensulfuron-methyl	21 - 29%	-	PSD 1991f
methomyl	thiodicarb	81.3% [b]	7 days	PSD 1992e
carbendazim	thiophanate-methyl	76%	3 weeks	EPA 2001d
DM-TM	tolclofos-methyl	10.5% [b]	90 days	PSD 1993d
DMST	tolyfluanid	~60% [b]	-	PSD 1995i
tralkoxydim metabolite 8	tralkoxydim	11.8% [b]	61 days	PSD 1993e
CGA 150829	triasulfuron	30% [b]	28 weeks	EU 2000b
triazamate metabolite II	triazamate	91% [b]	1 day	PSD 1998d
SAS 9256	triazoxide	21% [b]	64 days	PSD 1993f
triazine amine A	tribenuron methyl	91.1% [b]	14 days	PSD 1992f
3,5,6-trichloro-2-pyridinol	triclopyr	26%	<30 days	EPA 1998g
CGA-321113	trifloxystrobin	major [d]	-	PMRA 2004e
methyl saccahrin	triflusulfuron-methyl	84% [b]	29 days	PSD 1995j
trinexapac acid	trinexapac ethyl	major [d]	-	PSD 1995k
RPA 406341	triticonazole	20.2%	240 days	PSD 2000c

a - pesticide identified in the reference as the source of the transformation product

b - peak percentage formation of transformation product during study

c - time to peak transformation product formation

d - no precise formation data provided

2.5 Fate of Transformation Products in the Environment

Like all organic substances, once formed in the environment, a transformation product may be degraded by biotic and abiotic processes and may be transported between the different environmental compartments. A large body of data are available on the persistence and mobility of pesticide transformation products (Appendix A, Table A2 and A3 respectively).

2.5.1 Degradation in the Environment

Available data on the degradation rate constants of pesticide transformation products in different environmental compartments and under different conditions are provided in Appendix A, Table A2. Table 3 provides a summary of available transformation product degradation rate constant data determined in aerobic topsoil in the laboratory. Collated persistence data comprises disappearance time for 50% of a compound data (DT_{50}) and half-life data ($t_{½}$). DT_{50} is the time required for one-half the initial concentration of a compound to dissipate from a system were no assumption as to the rate equation is made, while half-life is the time taken for the concentration of a pesticide in a compartment to decline by one half were degradation can be described by first order kinetics (Holland 1996). The data are summarized in Figure 7 demonstrate that transformation products can be degraded by a range of processes. Fifteen of the transformation products (55%), are moderately (22 to 60 days) to very persistent (>60 days) in aerobic and anaerobic soil, as determined by the Soil Survey and Land Research Centre (SSLRC) soil persistence classification system (Hollis 1991).

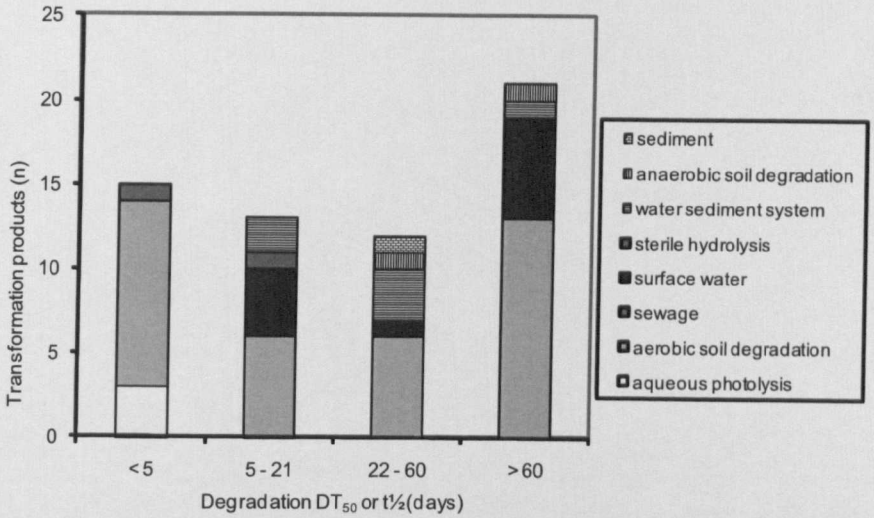

Figure 7. The degradation of pesticide transformation products, classified according to the SSLRC soil persistence classification

When degradation data for pesticide transformation products (Appendix A, Table A2) are compared to their parental compounds (Figure 8), 73.6% of the transformation products have equal or greater persistence than the pesticide. When summarizing these data, it is not possible to generalize that transformation products are more persistent than parent pesticide, because the data are probably skewed. Data pertaining to more persistent transformation products are probably more likely to be reported during a study while data concerning rapidly degrading transformation products is unlikely to be reported at all (Boxall et al. 2004). Although no generalizations can be made about a pesticide and its transformation products' persistence, these data include a number of transformation products that are more persistent than their parent pesticides. Therefore, these compounds can remain in the environment longer than the parent and have the potential to impact non-target organisms and/or move to other environmental compartments such as surface waters and groundwaters.

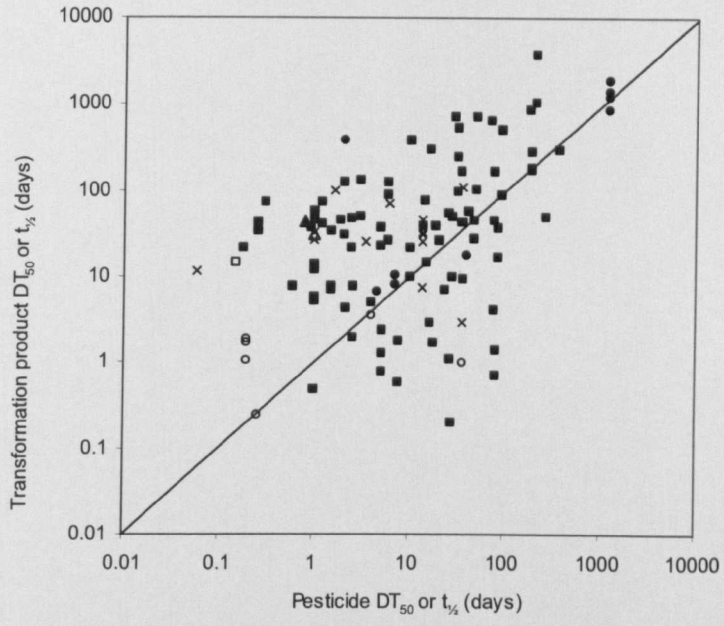

Figure 8. The comparative persistence of pesticides and their transformation products in various environmental media (aquatic photolysis (○), surface water (●), sterile hydrolysis (□), aerobic soil (■), anaerobic soil (Δ), sediment (▲) and sediment/water system (×) (The diagonal line represents equal persistence)

Table 3. Summary of transformation product degradation rate constants determined in aerobic topsoil in the laboratory

Transformation product	Parent pesticide [a]	Half-life / DT_{50}	Reference
3-chloroaryl alcohol (mean of isomers)	1,3-dichloropropene	0.1 - 0.6 days	EFSA 2006a
3-chloroacrylic acid (mean of isomers)	1,3-dichloropropene	0.7 - 19.8 days	EFSA 2006a
trans-3-chloroallylalcohol	*trans*-1,3-dichloropropene	0.4 – 1.4 days	Dijk 1974; Leistra et al. 1991
cis-3-chloroallylalcohol	cis-1,3-dichloropropene	1.2 – 4.2 days	Dijk 1974; Leistra et al. 1991
2,4-D	2,4-DB	2.3 - 17.1 days	EU 2002a
methamidophos	acephate	3.5 - 9.3 days	Sundaram 1993; PSD 1995a
2-chloro-2',6'-diethylacetanilide	alachlor	2.4 days	Fava et al. 2000
2-hydroxy-2',6'-diethylacetanilide	alachlor	0.8 days	Fava et al. 2000
2,6-diethylaniline	alachlor	1.3 days	Fava et al. 2000
aldicarb sulfone	aldicarb	18 - 154 days	APVMA 2001
aldicarb sulfoxide	aldicarb	20 - 53 days	APVMA 2001
BTS 27271	amitraz	67 - 82 days	EPA 1996a

Table 3. Summary of transformation product degradation rate constants determined in aerobic topsoil in the laboratory

Transformation product	Parent pesticide [a]	Half-life / DT_{50}	Reference
BTS 27919	amitraz	61 -117 days	EPA 1996a
dihydroxy anilazine	anilazine	21 - 45 days	PSD 1994b
deethylatrazine	atrazine	26 days	Solomon et al. 1996
deisopropylatrazine	atrazine	17 days	Solomon et al. 1996
diaminochloroatrazine	atrazine	19 days	Solomon et al. 1996
hydroxyatrazine	atrazine	121 days	Solomon et al. 1996
benalaxyl M1	benalaxyl	49 - 90 days	EU 2004c
benalaxyl M2	benalaxyl	66 - 118 days	EU 2004c
carbofuran	benfuracarb	11 - 44 days	PSD 1998a
3,5-dibromo-4-hydroxybenzamide	bromoxynil	0.47 - 5.2 days	EU 2004d
3,5-dibromo-4-hydroxybenzoic acid	bromoxynil	0.16 - 0.48 days	EU 2004d
3,5,-dibromo-4-hydroxybenzonitrile	bromoxynil octanoate	31 - 51 hours	EPA 1998b
tetrahydrophthalamide	captan	5.4 - 19.5 days	EPA 1999a
1-naphthol	carbaryl	14.93 days	Menon and Gopal 2003
N-phenyl-3-methyloxazoline-2,5-dione	carbetamide	21 - 23 days	Cantier et al. 1988
2-(phenylcarbamoyloxy)propionic acid	carbetamide	3.25 - 3.55 hours	Cantier et al. 1988
N-phenyl-2-hydroxypropionamide	carbetamide	25.4 - 27.9 days	Cantier et al. 1988
4-hydroxy-2,5,6-trichloroisophthalonitrile	chlorothalonil	6 – 130.6 days	PSD 2002; EU 2005b
R417888	chlorothalonil	121.1 days	EU 2005b
3-carbamyl-2,4,5-trichlorobenzoic acid	chlorothalonil	103 days	EU 2005b
3,5,6-trichloro-2-pyridinol	chlorpyrifos / chlorpyrifos-methyl / triclopyr	8 - 279 days	Tomlin 2000; APVMA 2000; Baskaran et al. 2003; EU 2005d
3-methoxy-3,5,6-trichloropyridine	chlorpyrifos / triclopyr	30 - >300 days	PMRA 1991; Belfroid et al. 1996; APVMA 2000
chlorthal-dimethyl mono-acid	chlorthal-dimethyl	2.8 days	Wettasinghe and Tinsley 1993
chlorthal-dimethyl di-acid	chlorthal-dimethyl	> 300 days	Wettasinghe and Tinsley 1993
clodinafop acid	clodinafop-propargyl	4.9 - 23 days	PSD 1995a; Tomlin 2000
cloquintocet acid	cloquintocet-mexyl	5 - 90 days	PSD 1995a
CCIM	cyazofamid	1.2 – 28.6 days	EU 2002c
CCIM-AM	cyazofamid	1 - 57 days	EU 2002c
CTCA	cyazofamid	17.7 - 395 days	EU 2002c
DCVA	cyfluthrin	12 - 62 days	EU 2002b
compound XV	*lambda*-cyhalothrin	7 - 16 days	EU 2001c
2,4,6-triamino-1,3,5-triazine melamine	cyromazine	263 - 1086 days	Belfroid et al. 1996
MTP	dacthal	2.8 days	EPA 1998c
methyl isothiocyanate	dazomet / metam-sodium	4 - 10 days	Belfroid et al. 1996; Roberts and Hutson 1999
decamethrinic acid	deltamethrin	0.7 - 9.1 days	EU 2002e
ethyl-m-hydroxyphenyl carbamate	desmedipham	9 - 27 days	PSD 1993b
diazoxon	diazinon	17 hours	PSD 1991b
3,6-dichlorosalicylic acid	dicamba	> 40 days	Pearson et al. 1996
diclofop acid	diclofop-methyl	6 - 63 days	PSD 1991c
omethoate	dimethoate	17 days	Belfroid et al. 1996
disulfoton sulfone	disulfoton	166 days	EPA 2002a
disulfoton sulfoxide	disulfoton	166 days	EPA 2002a
N'-(3,4-dichlorophenyl)-1-methylurea	diuron	217 - 1733 days	EPA 2003c
dipropylamine	EPTC	7 days	EPA 1999c
EPTC sulfoxide	EPTC	13 - 14 days	EPA 1999c
IN-KZ007	famoxadone	1.5 - 10.3 days	PMRA 2003e

Table 3. Summary of transformation product degradation rate constants determined in aerobic topsoil in the laboratory

Transformation product	Parent pesticide [a]	Half-life / DT_{50}	Reference
IN-KF015	famoxadone	1.2 days	PMRA 2003e
IN-JS940	famoxadone	6 -23 hours	PMRA 2003e
fenamiphos sulfoxide	fenamiphos	62 days	PSD 1990b
fenamiphos sulfone	fenamiphos	29 days	PSD 1990b
3-methyl-4-nitrophenol	fenitrothion	6 - 13 days	EPA 1995b; PMRA 2003d
fenoxaprop-ethyl acid	fenoxaprop-ethyl	5 - 14 days	PSD 1990c
5-hydroxy-XDE-570	florasulam	10 - 57 days	PMRA 2001b
fluazifop	fluazifop-p-butyl	3 - 16 weeks	PMRA 1988
fluazifop	fluazifop-butyl	3 - 16 weeks	PMRA 1988
MKH 6562 sulphonamide	flubcarbazone-sodium	> 400 days	PMRA 2000b
RH-5781	fluoroglycofen-ethyl	14 - 128 days	PSD 1992c
FBC 96912	fluquinconazole	448 days	PSD 1999a
4-amino-3,5-dichloro-6-fluoro-2-pyridinol	fluroxypyr	21 - 53 days	EU 1999
4-amino-3,5-dichloro-6-fluoromethoxypyridine	fluroxypyr	20 - 429 days	EU 1999
fluroxypyr	fluroxpyr-meptyl	< 7 days	Roberts 1998
phthalimide	folpet	17.2 days	PSD 1997a
AE F153745	formasulfuron	< 1 day	PMRA 2003g
dimethoate	formothion	7 - 40 days	Belfroid et al. 1996
formothioic acid	formothion	9 - 10 days	Belfroid et al. 1996
HOE 35950	glufosinate ammonium	4 - 42 days	PSD 1990e
3-methyl phosphinico-proprionic acid	glufosinate ammonium	7 - 165 days	PSD 1990e
aminomethylphosphonic acid	glyphosate / glyphosate trimesium	119 - 958 days	EPA 1993
1,2,4-triazole	hexaconazole	14 weeks	PMRA 1995
metsulfuron-methyl	iodosulfuron-methyl	20 - 99 days	PMRA 2004d
AE F161778	iodosulfuron-methyl	9.4 - 21.1 days	PMRA 2004d
AE F059411	iodosulfuron-methyl	119 - 269 days	PMRA 2004d
3,5-di-iodo-4-hydroxybenzamide	ioxynil / ioxynil octanoate	3.7 - 7.7 days	EU 2004e
3,5-di-iodo-4-hydroxybenzoic acid	ioxynil	<2 days	EU 2004e
ioxynil	ioxynil octanoate	1.5 - 2.5 days	EU 2004e
propargyl butyl carbamate	IPBC	4.3 days	PSD 1987; HSE 1994
RP 30228	iprodione	215 - 319 days	EU 2002j
desmethylisoproturon	isoproturon	22 - 65 days	EU 2002l
RPA 202248	isoxaflutole	24 - 96 days	PMRA 2000d
RPA 203328	isoxaflutole	289 - 977 days	PMRA 2000d
kresoxim-methyl acid	kresoxim-methyl	38 -131 days	PSD 1997b; Roberts and Hutson 1999; PMRA 2003b
MCPA acid	MCPA	24 days	PSD 1988c
MCPA	MCPB	24 days	EU 2005i
ethylenethiourea	mancozeb / maneb / metiram	2 hours – 2.5 days	Calumpang et al. 1993; PSD 2004b; EU 2005f; EU 2005g
ethyleneurea	mancozeb / maneb	4.8 - 7.6 days	Calumpang et al. 1993; EU 2005f; EU 2005g
ethylenebisisothiocyanide sulphide	maneb / metiram	0.09 – 0.8 days	EU 2005g
TDIT	metiram	0.3 - 0.9 days	EU 2005j
carbimid	metiram	0.009 - 0.9 days	EU 2005j
HOE 113225	mefenpyr-diethyl	9 days	PSD 1999a
HOE 094270	mefenpyr-diethyl	135 days	PSD 1999a
2-ethyl-6-methylaniline	metolachlor	1.7 days	Fava et al. 2000
IN-A4098	metsulfuron-methyl	210 days	EU 2000a
IN-D5803	metsulfuron-methyl	<< 1 month	EU 2000a
ADMP	nicosulfuron	2 - 7 days	PSD 2000b
ASDM	nicosulfuron	95 - 113 days	PSD 2000b
AUSN	nicosulfuron	53 - 91 days	PSD 2000b

Table 3. Summary of transformation product degradation rate constants determined in aerobic topsoil in the laboratory

Transformation product	Parent pesticide [a]	Half-life / DT_{50}	Reference
UCSN	nicosulfuron	128 days	PSD 2000b
phorate sulfoxide	phorate	65 - 137 days	PMRA 2003a
phorate sulfone	phorate	65 - 137 days	PMRA 2003a
CL 153815	picolinafen	30 - 77 days	PMRA 2003h
1,2,4-triazole	propiconazole	2 - 12 days	EU 2003e
CGA 118 245	propiconazole	<1 day	EU 2003e
propylene urea	propineb	4 - 93 days	EU 2003f
propylenethiourea	propineb	1.5 - 2.6 days	EU 2003f
2-(3,5-dichlorophenyl)-4,4-dimethyl-5-methyleneoxazoline	propyzamide	25.8 - 37.9 days	EU 2003h
N-(1,1-dimethylacetonyl)-3,5-dichlorobenzamide	propyzamide	12.4 - 16.7 days	EU 2003h
BH518-2	quinmerac	17 - 1080 days	PSD 1998c
BH518-5	quinmerac	4 - 3850 days	PSD 1998c
anilino acid	tau-fluvalinate	5.7 – 7.1 days	PSD 1997d
2,6-di-*tert*-butyl-4-methylphenyl carbamate	terbutol	291 days	Suzuki et al. 2001
2,6-di-*tert*-butyl-4-carboxyphenyl *N*-methylcarbamate	terbutol	173 days	Suzuki et al. 2001
2,6-di-*tert*-butyl-4-carboxyphenyl carbamate	terbutol	184 days	Suzuki et al. 2001
thifensulfuron acid	thifensulfuron-methyl	2.2 - >365 days	EU 2001e
O-desmethyl thifensulfuron-methyl	thifensulfuron-methyl	< 2.9 - 15.3 days	EU 2001e
thiophene sulfonimide	thifensulfuron-methyl	9.6 - 96.6 days	EU 2001e
IN-A4098	thifensulfuron-methyl	22 - 176 days	EU 2001e
2-ester-3-sulfonamide	thifensulfuron-methyl	6 - 7 days	EU 2001e
methomyl	thiodicarb	45 days	EPA 1998f
carbendazim	thiophanate-methyl	39.8 - 320 days	EPA 2001d; EU 2005k
tridimenol	triadimefon	> 2 years	Bromilow et al. 1999
CGA 150829	triasulfuron	159 - 289 days	EU 2000b
triazamate metabolite II	triazamate	1.7 - 70 days	PSD 1998d
triazine amine A	tribenuron methyl	110 - 240 days	PSD 1991d; EFSA 2004
IN-A4098	tribenuron-methyl	22 - 39 days	EFSA 2004
saccahrin	tribenuron-methyl	230 days	EFSA 2004
2-butoxyethanol	triclopyr butoxyethyl ester	0.058 - 0.375 days	EPA 1998g
CGA-321113	trifloxystrobin	250 - 350 days	PMRA 2004e
trinexapac acid	trinexapac ethyl	1.1 - 21.4 days	PSD 1995k
RPA 406341	triticonazole	165 - 330 days	PMRA 2004b
RPA 407922	triticonazole	0.5 - 1.1 days	PMRA 2004b

a - pesticide identified in the reference as the source of the transformation product

2.5.2 Routes into environmental waters for non-agricultural pesticides and transformation products

The monitoring and measurement of pesticides and their transformation products is understandably dominated by the occurrence of agricultural herbicides in agricultural areas. However, pesticides are also widely used in other areas which could be an important source of transformation products in environmental waters. Non-agricultural pesticide market sectors include industrial, commercial,

government and domestic (Donaldson et al. 2002). Due to the method or site of application, pesticides used in these sectors can have the potential for direct entry into surface waters. Following herbicidal application to hard surfaces such as asphalt and concrete, more than half of applied atrazine and diuron can be lost to the highway drainage system during the first 5mm of rainfall (Ramwell et al. 2002). In the UK, five herbicides (2,4-D, dichlobenil, diquat, glyphosate and terbutryn) and one plant growth regulator (maleic hydrazide) are approved for use in or near water (Whitehead 2004). Obviously, this method of application can provide the pesticides with a direct entry route into surface waters where they could degrade and produce transformation products in relatively large quantities. In contrast to agricultural streams, the total insecticide concentration in urban streams exceeds that of the total herbicide concentration. However, no insecticidal transformation products were detected in urban streams when sampled during one study, with DEA the only herbicide transformation product identified (Hoffman et al. 2000).

2.5.3 Effects of climate and season

One of the dominant factors affecting the occurrence of transformation products in environmental waters (surface and ground) is climatic conditions. High concentrations of triazine transformation products (DEA and DIA) are identified in agricultural ditches if there is heavy rainfall soon after atrazine application (Thurman et al. 1994). Moreover, if dry summer conditions follow the spring application of atrazine, then the first large rainfall event can 'flush' transformation products from the soil resulting in peak concentrations in agricultural ditches. It is hypothesized that during the summer, transformation product quantities increase and are stored in soil which are then readily transported to surface waters by heavy rainfall. Metolachlor ESA and metolachlor OA concentrations in agricultural ditch samples peaked in the first flow event in November following a dry summer. These concentrations quickly declined once the stored transformation products had been flushed out of the soil (Phillips et al. 1999). These large peak concentrations are observed in

subsequent surface waters such as streams and rivers (Albanis and Hela 1998; Clark et al. 1999).

2.5.4 Mobility in the environment

One of the most important physico-chemical properties of a transformation product for determining whether it will be mobile is its organic carbon normalized sorption coefficient (K_{oc}). The data collected during this review for transformation products on K_{oc}, K_d, K_f and K_{foc} are provided in Appendix A, Table A3, K_{oc} data are summarized in Table 4. This property is a measure of the extent to which a chemical will adsorb to the soil. Compounds with a high K_{oc} bind to the organic material in soil and hence, have a low degree of mobility. Boxall et al. (2004) investigated the relationship between the sorption of transformation products and their pesticidal parents from K_{oc} data collected from numerous databases. Approximately one third of the transformation products had a K_{oc} value of at least an order of magnitude lower than the corresponding parent compound. During this study, sorption data were collated from studies where both the parent and the transformation product K_{oc} were determined. This was done so that comparative analysis would not be affected by inter-laboratory variability. When K_{oc} is determined experimentally, it is usual to use a number of different soils with varying properties, e.g. pH, clay content, % organic carbon content. This usually provides a range of K_{oc} values for each compound from the range of soil types used. A comparison was undertaken between the mobility of a pesticide to that of its transformation product(s), the minimum K_{oc} value for each compound derived in a study were used (Figure 9). Seventeen of the transformation products had a K_{oc} greater than the parent pesticide whilst 21 pesticides had a K_{oc} greater than their transformation product. When the mobility of the transformation products (including those without pesticide comparative data) are classified according to the SSLRC mobility classification (Hollis 1991), 50% of the transformation products are categorized as mobile to very mobile (K_{oc} <75) with 35.5% categorized as slightly mobile (K_{oc} 75 - 499).

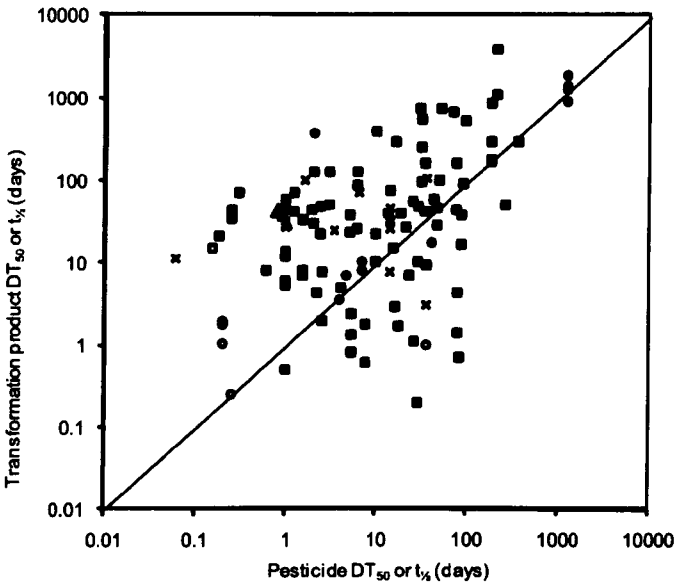

Figure 9. The comparative sorption of transformation products and their parent pesticides

The lower sorption coefficients and increased solubility of two atrazine transformation products, (DEA and DIA), indicate that they have a greater potential to move through the soil profile to groundwater than the parent compound (Mills and Thurman 1994). The rate of degradation and the sorptive behavior of pesticides and their transformation products will determine their persistence in soil and their mobility to surface and ground waters. Transformation products of the triazine herbicides, cyanazine (Reddy et al. 1997) and atrazine (Krutz et al. 2003), show equal or lower levels of sorption to a range of soil types than the parent compound. This could increase their mobility and thus, the potential to enter surface and ground waters. Moreover, the sorption of transformation products of the chloroacetamide herbicides alachlor and metolachlor is approximately equal to or less than that for the parent compounds. However, the rapid rate of degradation (<2.4 days) for all the transformation products of these two herbicides will influence the extent of their persistence and hence mobility (Fava et al. 2000).

Table 4. Summary containing collated mean values for organic carbon partition coefficients (K_{oc}) of pesticide transformation products

Transformation product	Parent pesticide	K_{oc} range	K_{oc} mean	n	Reference(s)
(EZ)-3-chloroacrylic acid	1,3-dichloropropene	<1-17.5	3.8		EFSA 2006a
(EZ)-3-chloroallyl alcohol	1,3-dichloropropene	5.3-11.9	9.4		EFSA 2006a
2,4-dichlorophenol	2,4-D		108[a]		Haberhauer et al. 2000; Fava et al. 2005
2,4-D[e]	2,4-DB	31-74	47.8	5	EU 2002a
R1	acequinocyl	1175-22813	95264.3	3	PMRA 2007a
IM-1-5	acetamiprid	453-563	508	2	EU 2004a
2,6-diethylaniline	alachlor		357[a]		Fava et al. 2000
2-chloro-2',6'-diethylacetanilide	alachlor		148[a]		Fava et al. 2000
2-hydroxy-2',6'-diethylacetanilide	alachlor		45[a]		Fava et al. 2000
alachlor ethane sulfonic acid	alachlor	15-182	98.5	2	APVMA 2001; Aga and Thurman 2001
3-phenoxybenzoic acid	alpha-cypermethrin		73[c]		EU 2004b
2-amino-4,6-dimethoxypyrimidine	amidosulfuron		29[a]		PSD 1994a
4,6-dihydroxypyrimidin-2-yl-urea	amidosulfuron		0.4[a]		PSD 1994a
HOE 101630[e]	amidosulfuron		3[a]		PSD 1994a
deethylatrazine	atrazine	10-67	38.9	18	Brouwer et al. 1990; PSD 1992a; Mills and Thurman 1994; Solomon et al. 1996; APVMA 1997a; Steinheimer and Scoggin 2001; EPA 2003b
deisopropylatrazine	atrazine & simazine		58.6	17	Brouwer et al. 1990; PSD 1992a; PSD 1992d; Mills and Thurman 1994; Solomon et al. 1996; APVMA 1997a; Steinheimer and Scoggin 2001; EPA 2003b
diaminochlorotriazine	atrazine & simazine	31-76	55	4	PSD 1992d; Solomon et al. 1996; APVMA 1997a; EPA 2003b
hydroxyatrazine	atrazine	103-13797	1677.6	12	Brouwer et al. 1990; PSD 1992a; Solomon et al. 1996; APVMA 1997a; EPA 2003b
reference compound 2	azoxystrobin	33-770	328.7	6	PMRA 2000a; PMRA 2007d
reference compound 28	azoxystrobin	90-810	285	6	PMRA 2000a; PMRA 2007d
reference compound 30	azoxystrobin	40-250	106	6	PMRA 2000a; PMRA 2007d
benalaxyl M1	benalaxyl	151-455	375.6	3	EU 2004c
benalaxyl M2	benalaxyl	80-756	321	3	EU 2004c
carbofuran	benfuracarb	17-28	22	4	EFSA 2006b
N-methyl bentazone	bentazone	250-350	300	2	Gaston et al. 1996
DCVA[e]	beta-cyfluthrin	14-356	133.7	3	EU 2002b
D1989	bifenazate	3725-3962	3864	3	EU 2005a
			6189[d]		EU 2005a
D3598	bifenazate		8710[b]		EU 2005a
THPAM	captan	3.8-110	45.2	6	EFSA 2006c
1-naphthol	carbaryl		245[a]		EFSA 2006d
4-hydroxy-2,5,6-trichloroisophthalonitrile	chlorothalonil	95-1100	467.5	18	PSD 2002; EU 2005b
R417888	chlorothalonil	6-17	10	6	EU 2005b
3,5,6-trichloro-2-methoxypyridine	chlorpyrifos & chlorpyrifos-methyl	565-1308	888	5	EU 2005d; EU 2005e
		27-389	165	29	APVMA 2000
		77-242	148.5	4	EPA 1998g; EPA 1999d; EU 2005d; EU 2005e
		67.2-316.3	172.4	5	EFSA 2005d; EU 2005d; EU 2005e
chloroacid cyanazine	cyanazine	7-11	9.7	4	Reddy et al. 1997

Table 4. Summary containing collated mean values for organic carbon partition coefficients (K_{oc}) of pesticide transformation products

Transformation product	Parent pesticide	K_{oc} range	K_{oc} mean	n	Reference(s)
cyanazine amide	cyanazine	16-75	45.3	4	Reddy et al. 1997
desmethylpropanenitrile cyanazine	cyanazine	89-133	105.3	4	Reddy et al. 1997
deethylcyanazine	cyanazine	26-82	62.3	4	Reddy et al. 1997
hydroxyacid cyanazine	cyanazine	11-130	75.5	4	Reddy et al. 1997
2,4-dichloroaniline	cyclanilide	349-681	508.8	4	EU 2001a
cyhalofop-acid	cyhalofop-butyl	176-195	185.5	2	EU 2002d
cyhalofop-diacid	cyhalofop-butyl	27-401	149.3	4	EU 2002d
3,6-dichlorosalicylic acid	dicamba		504		Pearson et al. 1996
2,6-dichlorobenzoic acid	dichlobenil		<18[a]		Fava et al. 2005
diclofop acid	diclofop-methyl	191-334	269.3	3	PSD 1991c
M23	dimethenamid & dimethenamid-P	3.5-17.2	7.7	6	EU 2003a; EFSA 2005a
M27	dimethenamid & dimethenamid-P	0.0-14.4	6.7	6	EU 2003a; EFSA 2005a
endosulfan sulphate	endosulfan		<12[a]		Fava et al. 2005
IN-JS940	famoxadone	33-591	330	4	EU 2002f; PMRA 2003e
IN-KF015	famoxadone	130-1300	505	4	EU 2002f; PMRA 2003e
IN-KZ007	famoxadone	1238-34423	13705	4	EU 2002f; PMRA 2003e
ASTCA	florasulam	24-110	53.1	10	EU 2002g
DFP-ASTCA	florasulam	27-159	83	10	EU 2002g
CGA 265378	fludioxonil	0.65-0.83	0.75	4	EFSA 2007a
JV460	flupyrsulfuron-methyl	65-106	83.3	3	EU 2001b
KC576	flupyrsulfuron-methyl	22-48	36.7	3	EU 2001b
KY374[e]	flupyrsulfuron-methyl	3-39	16.5	6	EU 2001b
TFAA	flurtamone	3.2-27.5	22.9		EU 2003b
IN-F7321	flusilazole	164-822	532.3	4	EU 2007a
IN-H9933	flusilazole	8-22	16.5	4	EU 2007a
AE F153745	formasulfuron	35-63	49.3	3	EU 2002h; PMRA 2003g
metabolite M01	fuberidazole	13-15	14	3	EFSA 2007b
HOE 35956	glufosinate ammonium		16		PSD 1990e
IN-JT333	indoxacarb	8200-25000	17300	4	Strek et al. 2007
AE F161778	iodosulfuron-methyl		~60		EU 2003c
PMPA	iprovalicarb	118-575	290.3	4	EU 2002k
RPA 202248	isoxaflutole	94-159	129.8	4	PMRA 2000d
RPA 203328	isoxaflutole	47-100	80	4	PMRA 2000d
			23[d]		PMRA 2000d
kresoxim-methyl acid	kresoxim-methyl	17-69	37.4	4	PSD 1997b; EU 1998; PMRA 2003b
compound XV	*lambda*-cyhalothrin	36000-61000	44000	6	EU 2001c
2-methyl-4-chlorophenol	MCPA		93[a]		Haberhauer et al. 2000; Fava et al. 2005
MCPA[e]	MCPB	10-157	74	8	EU 2005i
methiocarb sulfoxide	methiocarb		31.3		EFSA 2006e
2-ethyl-6-methylaniline	metolachlor		197		Fava et al. 2000
metolachlor ethane sulfonic acid	metolachlor		195		Aga and Thurman 2001
CGA-51202	metolachlor & S-metolachlor	2.82-62	12.2	7	EPA 1995d; EU 2004g

Table 4. Summary containing collated mean values for organic carbon partition coefficients (K_{oc}) of pesticide transformation products

Transformation product	Parent pesticide	K_{oc} range	K_{oc} mean	n	Reference(s)
IN-A4098	metsulfuron-methyl, thifensulfuron-methyl & tribenuron-methyl	17-226	98	7	EU 2000a; EU 2001e; EFSA 2004
saccharin	metsulfuron-methyl & propoxycarbazone	5.7-10.6	8.9	4	EU 2000a
		4.6-15.5	5.2[c]	5	EU 2003g
hexamethyleneimine	molinate	226-603	426.2	5	EU 2003d
molinate sulfoxide	molinate	93-234	168.8	5	EU 2003d
UCSN	nicosulfuron	1.1-5.6	2.7	4	PSD 2000b; PMRA 2008
RP017272	oxadiargyl		856		EU 2002m
RP025496	oxadiargyl		468		EU 2002m
IN-A2213	oxamyl	4-11	7	5	EFSA 2005b
IN-D2708	oxamyl	2-10	6	5	EFSA 2005b
IN-N0079	oxamyl	2-25	8	5	EFSA 2005b
C1801	oxasulfuron	54-213	146	3	EU 2002n
CGA 27913	oxasulfuron	3-6	4	3	EU 2002n
MET-42	pethoxamid	1.29-2.97	2.13	2	EU 2006a
CL 153815	picolinafen	160-783	440	4	EU 2002o; PMRA 2003h
M2	pinoxaden	4.2-27	13.1	5	PMRA 2006a
M3	pinoxaden	23-48	31.6	5	PMRA 2006a
propachlor oxanilic acid	propachlor	2-10	6.8	4	EPA 1998e
propachor sulfonic acid	propachlor	3-7	5.3	4	EPA 1998e
3,4-dichloroaniline	propanil		258		Fava et al. 2005
propylene urea	propineb	13-26	18	4	EU 2003f
4-hydroxy saccharin	propoxycarbazone	456.9-2872.7	2033.8	5	EU 2003g
N-methyl propoxy triazolinone	propoxycarbazone	8.9-75.5	20.6	5	EU 2003g
N-methyl propoxy triazolinone amide	propoxycarbazone	10.4-551.5	99.9	5	EU 2003g
2-(3,5-dichlorophenyl)-4,4-dimethyl-5-methyleneoxazoline	propyzamide	993-3910	1894	6	EU 2003h
N-(1,1-dimethylacetonyl)-3,5-dichlorobenzamide	propyzamide	96-210	153	6	EU 2003h
prosulfocarb sulfoxide	prosulfocarb	61-88	70.7	3	EFSA 2007c
CGA 150829	prosulfuron & triasulfuron	55-281	144	4	EU 2000b; EU 2002p
CGA 159902	prosulfuron	48-96	77	4	EU 2002p
CGA 300406	prosulfuron	43-126	66.8	4	EU 2002p
CGA 325025	prosulfuron	60-238	123	4	EU 2002p
CGA 325030	prosulfuron	18-41	21	4	EU 2002p
CGA 32508	prosulfuron	11-31	20	5	EU 2002p
CGS 349707	prosulfuron	37-52	45	3	EU 2002p
prothioconazole-thiazocine	prothioconazole		129		PMRA 2007e
CGA 354743	S-metolachlor	3-22	9[c]	7	EU 2004g
CGA 376944	S-metolachlor	8-12	10[c]	3	EU 2004g
CGA 40172	S-metolachlor	143-204	182[c]	3	EU 2004g
CGA 41507	S-metolachlor	81.3-93.8	84.9[c]	3	EU 2004g
BAJ 2740-dioxoketone	spirodiclofen		3720		PMRA 2006b
M09	spiromesifen		3		EFSA 2007d
		1042.4-8278	4660.2	2	PMRA 1998; EU 2002q
sulphonamide	sulfosulfuron	60.9-260.5	163	4	PMRA 1998; EU 2002q

Table 4. Summary containing collated mean values for organic carbon partition coefficients (K_{oc}) of pesticide transformation products

Transformation product	Parent pesticide	K_{oc} range	K_{oc} mean	n	Reference(s)
2,3,5,6-tetrachloroaniline	tecnazene	5102-26700	12662.3	4	PSD 1995h
DP-1	tepraloxydim	48-1107	252.5	6	PMRA 2004a; EU 2004h
		63-4193	791.3	6	EU 2004h
M34	thiacloprid	2.94-6.27	5.02	4	EU 2004i
CGA 322704	thiamethoxam	63-77	70	3	EU 2006b
CGA 355190	thiamethoxam	37.6-187.5	91.5	6	EU 2006b; PMRA 2007b
NOA 407475	thiamethoxam	433-1550	761.2	6	EU 2006b; PMRA 2007b
IN-L9225	thifensulfuron-methyl	6.9-13.5	11.2	3	EU 2001e
IN-L9226	thifensulfuron-methyl	34-199	111	3	EU 2001e
carbendazim	thiophanate-methyl		2100		EPA 2001d
DM-TM	tolclofos-methyl	11-22.2	15	3	EFSA 2005c
triazamate metabolite II	triazamate	23-314	102	5	PSD 1998d
triazamate metabolite III	triazamate	34-493	150.4	5	PSD 1998d
triazamate metabolite IV	triazamate	28-376	115	5	PSD 1998d
IN-00581	tribenuron-methyl	12-20	15	3	EFSA 2004
IN-L5296	tribenuron-methyl	53-138	89	3	EFSA 2004
NOA 413161	trifloxystrobin		4.2		EU 2003i
RPA 406341	triticonazole	61-163	122.5	4	PMRA 2004b
RPA 407922	triticonazole	467-1305	761	4	PMRA 2004b

[a] – determined by HPLC

[b] – determined by column leaching

[c] – median value

[d] – sediment

[e] – pH dependent adsorption identified

2.6 Occurrence in the Environment

Whether pesticides are present in environmental waters (surface water and groundwater) following their agricultural application is determined by a large number of factors including climatic conditions, e.g. rainfall and temperature, mass transfer processes, chemical properties, e.g. solubility, degradation and sorption, agricultural practices, e.g. application rate, tillage practices and land use, specific location properties, e.g. soil properties, hydrological properties and topography, application methods, e.g. foliar application and soil incorporation, and product formulation (Lerch and Blanchard 2003). All of these factors are also important in determining whether transformation products are present in surface water and groundwater. However the importance of these factors in determining the fate of transformation products when compared to pesticides

will differ. If a pesticide degrades rapidly in soil, then it is unlikely that this compound will be detected in environmental waters; however, its transformation products could form in relatively large quantities. Therefore, rapid pesticide degradation is an advantageous property in preventing pesticide contamination but possibly disadvantageous for preventing its transformation products from entering environmental waters. When the chloroacetamide herbicides are applied at the same rate during normal agricultural practice, the ESA transformation product of alachlor is present at higher concentrations than metolachlor ESA in soil. This difference is due to the relatively longer half-life of metolachlor (15.5 d) in soil and thus slower formation of metolachlor ESA when compared to alachlor (8 d) (Aga and Thurman 2001). However, pesticide usage will be of greater importance in determining the degree of transformation product occurrence in environmental waters. In the US in 1997, 5.8 - 7.3 million kg of alachlor was used in the agricultural sector compared to 28.6 - 31.3 million kg of metolachlor (Kiely et al. 2004). Therefore even though the relative formation of alachlor ESA is greater than metolachlor ESA, the higher usage of metolachlor in the agricultural sector will mean that metolachlor transformation products will be detected at higher concentrations and more frequently than alachlor. Monitoring studies of surface and ground waters identify metalchlor ESA detected at higher concentrations and more frequently than the alachlor ESA (Kolpin et al. 1998; Kalkhoff et al. 1998).

Pesticide transformation products have been detected in numerous environmental compartments: soil, soil leachate, tile drains, surface waters including agricultural ditches, streams, rivers, reservoirs, canals, ponds, lakes and estuaries, groundwater, sediment, air including gaseous, and particulate phases and rain. Appendix A, Table A4 provides a summary of these occurrences in soil, surface water, groundwater, raw source water, and finished drinking water (occasions where transformation products were anaylsed and not detected are also included). Table 5 provides maximum concentration of transformation products identified in river water and groundwaters.

Table 5. A summary of maximum concentrations of pesticide transformation products identified in surface waters (rivers only) and groundwater

Transformation product	Parent pesticide [a]	Concentration	Limit of detection	Country	Reference
Surface water (Rivers)					
acetochlor oxanilic acid	acetochlor	ND - 0.15 µg L^{-1}	0.01 µg L^{-1}	USA	Ferrer et al. 1997
alachlor ethane sulfonic acid	alachlor	1.55 - 4.75 µg L^{-1} [c]	0.1 µg L^{-1}	USA	Battaglin and Goolsby 1999
alachlor oxanilic acid	alachlor	ND - 0.21 µg L^{-1}	0.01 µg L^{-1}	USA	Ferrer et al. 1997
2,6-diethylaniline	alachlor	ND - 0.924 µg L^{-1}	5 ng L^{-1}	USA	Pereira and Rostad 1990
2-chloro-2',6'-diethylacetanilide	alachlor	ND - 0.35 µg L^{-1}	5 ng L^{-1}	USA	Pereira and Rostad 1990
2-hydroxy-2',6'-diethylacetanilide	alachlor	ND - 0.9 µg L^{-1}	5 ng L^{-1}	USA	Pereira and Rostad 1990
8-hydroxy-bentazone	bentazone	ND - 27 µg L^{-1}	2 ng L^{-1}	Italy	Lagana et al. 2002
cyanazine amide	cyanazine	0.47 - 0.57 µg L^{-1} [c]	0.05 µg L^{-1}	USA	Battaglin and Goolsby 1999
deethylcyanazine	cyanazine	< 0.05 µg L^{-1} [c]	0.05 µg L^{-1}	USA	Battaglin and Goolsby 1999
deethylcyanazine amide	cyanazine	< 0.05 µg L^{-1} [c]	0.5 µg L^{-1}	USA	Battaglin and Goolsby 1999
deethylatrazine	atrazine and propazine	12 - 28 µg L^{-1} [c]	-	USA	Solomon et al. 1996
deisopropylatrazine	atrazine, cyanazine and simazine	4.9 - 15 µg L^{-1} [c]	-	USA	Solomon et al. 1996
p,p'-DDE	DDT	4 ng L^{-1} [b]	0.3 ng L^{-1}	USA	Liu et al. 2002
dimethenamid ethane sulfonic acid	dimethenamid	0.05 µg L^{-1} [c]	0.03 µg L^{-1}	USA	Zimmerman et al. 2002
dimethenamid oxanilic acid	dimethenamid	0.05 µg L^{-1} [c]	0.02 µg L^{-1}	USA	Zimmerman et al. 2002
endosulfan sulphate	endosulfan	6 ng L^{-1}	0.3 ng L^{-1}	USA	Liu et al. 2002
flufenacet ethane sulfonic acid	flufenacet	0.06 µg L^{-1} [c]	0.01 µg L^{-1}	USA	Zimmerman et al. 2002
flufenacet oxanilic acid	flufenacet	0.05 µg L^{-1} [c]	0.07 µg L^{-1}	USA	Zimmerman et al. 2002
metolachlor oxanilic acid	metolachlor	ND - 0.29 µg L^{-1}	0.01 µg L^{-1}	USA	Ferrer et al. 1997
metolachlor ethane sulfonic acid	metolachlor	0.33 - 1.82 µg L^{-1}	0.01 µg L^{-1}	USA	Ferrer et al. 1997
3,4-dichloroaniline	propanil	ND - 26 ppb	0.05 ppb	USA	PSD 1988b
Groundwater					
3-chloroallyl alcohol	1,3-dichloropropene	trace - 13.5 ppb	0.05 ppb	USA	EPA 1998a
3-chloroacrylic acid	1,3-dichloropropene	trace - 8.79 ppb	0.05 ppb	USA	EPA 1998a
2,4-dichlorophenol	2,4-D	4 µg L^{-1} [b]	-	Denmark	Helweg et al. 2002
acetochlor ethane sulfonic acid	acetochlor	8.6 µg L^{-1} [b]	0.1 µg L^{-1}	USA	Kolpin et al. 1996a
acetochlor oxanilic acid	acetochlor	11.5 µg L^{-1} [b]	0.2 µg L^{-1}	USA	Kolpin et al. 2000
α-N-[(2'-6'-diethylphenylamino)ethanol	alachlor	< 2 - 480 ng L^{-1}	-	USA	Potter and Carpenter 1995
2-chloro-2'-ethyl-6'-ethyl-N-(methoxymethyl)acetanilide	alachlor	< 2 - 310 ng L^{-1}	-	USA	Potter and Carpenter 1995
2'-acetyl-6'-ethylacetanilide	alachlor	28 - 120 ng L^{-1}	-	USA	Potter and Carpenter 1995
2'-acetyl-6'-ethyl-N-methoxymethyl)acetanilide	alachlor	68 - 240 ng L^{-1}	-	USA	Potter and Carpenter 1995
2-hydroxy-2',6'-diethyl-N-methyl)acetanilide	alachlor	< 2 - 130 ng L^{-1}	-	USA	Potter and Carpenter 1995

Table 5. A summary of maximum concentrations of pesticide transformation products identified in surface waters (rivers only) and groundwater

Transformation product	Parent pesticide [a]	Concentration	Limit of detection	Country	Reference
2-hydroxy-2',6'-diethyl-N-methoxymethyl)acetanilide	alachlor	< 2 - 100 ng L^{-1}	-	USA	Potter and Carpenter 1995
2,6-diethylaniline	alachlor	0.085 µg L^{-1} [b]	0.003 µg L^{-1}	USA	Kolpin et al. 1998
2',6'-diethylacetanilide	alachlor	< 2 - 130 ng L^{-1}	-	USA	Potter and Carpenter 1995
2',6'-diethylformanilide	alachlor	< 2 - 87 ng L^{-1}	-	USA	Potter and Carpenter 1995
7-ethylindoline	alachlor	< 2 - 35 ng L^{-1}	-	USA	Potter and Carpenter 1995
alachlor ethane sulfonic acid	alachlor	0.06 - 9.32 µg L^{-1}	0.05 µg L^{-1}	USA	Aga et al. 1994
alachlor oxanilic acid	alachlor	33.4 µg L^{-1} [b]	0.2 µg L^{-1}	USA	Kolpin et al. 2000
N-(2,6-diethylphenyl) methylene	alachlor	< 2 - 10 ng L^{-1}	-	USA	Potter and Carpenter 1995
N-(2,6-diethylphenyl)-N-(methoxymethyl)acetamide	alachlor	100 - 550 ng L^{-1}	-	USA	Potter and Carpenter 1995
deethylatrazine	atrazine	5 µg L^{-1}	0.02 µg L^{-1}	USA	Adams and Thurman 1991
deisopropylatrazine	atrazine, cyanazine, simazine	1.17 µg L^{-1} [b]	0.05 µg L^{-1}	USA	Kolpin et al. 1996b
deisopropylhydroxyatrazine	atrazine, cyanazine, simazine	0.04 µg L^{-1} [c]	0.04 µg L^{-1}	USA	Steinheimer and Scoggin 2001
hydroxyatrazine	atrazine	1.3 µg L^{-1} [b]	0.2 µg L^{-1}	USA	Kolpin et al. 2000
2-aminobenzimidazole	carbendazim [a]	0.03 µg L^{-1} [b]	-	Spain	Hernandez et al. 2008
carbofuran-7-PhOH-3CO	carbofuran	0.06 µg L^{-1}	-	Spain	Hernandez et al. 2008
3-carbamyl-2,4,5-trichlorobenzoic acid	chlorothalonil	2 - 12.6 µg L^{-1}	2 µg L^{-1}	USA	EPA 1999b
3-cyano-6-hydroxy-2,4,5-trichlorobenzamide	chlorothalonil	2 - 5 µg L^{-1}	2 µg L^{-1}	USA	EPA 1999b
4-hydroxy-2,5,6-trichloroisophthalonitrile	chlorothalonil	3.6 µg L^{-1}	2 µg L^{-1}	USA	EPA 1999b
3-cyano-2,4,5,6-tetrachlorobenzamide	chlorothalonil	2.8 µg L^{-1}	2 µg L^{-1}	USA	EPA 1999b
3,4-dichloroaniline	chlorpyrifos, diuron, linuron, propanil	<0.025 µg L^{-1} [b]	-	Spain	Hernandez et al. 2008
cyanazine amide	cyanazine	0.64 µg L^{-1} [b]	0.05 µg L^{-1}	USA	Kolpin et al. 2000
chlorthal-dimethyl di-acid	chlorthal-dimethyl	2.22 µg L^{-1} [b]	0.01 µg L^{-1}	USA	Kolpin et al. 1996b
p,p'-DDE	DDT	0.03 µg L^{-1} [b]	0.03 µg L^{-1}	-	Kolpin et al. 1996b
2,6-dichlorbenzamide	diclobenil	180 ppb	-	Netherlands	EPA 1998d
endosulfan sulphate	endosulfan	ND - 1.4 ppb	0.005 ppb	USA	EPA 2002c
AMPA	glyphosate	1.6 µg L^{-1} [b]	-	Denmark	Helweg et al. 2002
α-HCH	gamma-HCH	0.059 µg L^{-1} [b]	0.002 µg L^{-1}	USA	Kolpin et al. 1998
monodesmethyl isoproturon	isoproturon	~0.05 µg L^{-1}	≤ 0.05 µg L^{-1}	France	Baran et al. 2008
didesmethylisoproturon	isoproturon	ND	≤ 0.05 µg L^{-1}	France	Baran et al. 2008
metolachlor ethane sulfonic acid	metolachlor	15.2 µg L^{-1}	-	USA	Steele et al. 2008
metolachlor oxanilic acid	metolachlor	15.3 µg L^{-1} [b]	0.2 µg L^{-1}	USA	Kolpin et al. 2000
2,4-bis(isopropylamino)-6-hydroxy-s-triazine	prometryn	0.61 ppb	-	USA	EPA 1996c
hydroxysimazine	simazine	0.15 µg L^{-1} [c]	0.04 µg L^{-1}	USA	Steinheimer and Scoggin 2001

Table 5. A summary of maximum concentrations of pesticide transformation products identified in surface waters (rivers only) and groundwater

Transformation product	Parent pesticide [a]	Concentration	Limit of detection	Country	Reference
desethyl-2-hydroxyterbuthylazine	terbuthylazine	0.21 µg L^{-1} [b]	-	Spain	Hernandez et al. 2008
desethylterbuthylazine	terbuthylazine	1.42 µg L^{-1} [b]	-	Spain	Hernandez et al. 2008
hydroxyterbuthylazine	terbuthylazine	0.15 µg L^{-1} [b]	-	Spain	Hernandez et al. 2008
desethylterbumeton	terbumeton	1.62 µg L^{-1} [b]	-	Spain	Hernandez et al. 2008
methomyl	thiodicarb	0.1 -0.4 ppb	-	USA	EPA 1998f

a - pesticide identified in the reference as the source of the transformation product

b - peak concentration during study

c - median or mean concentration

2.6.1 Soil

Transformation products can be expected to be present in soil following the application of the parent pesticide if it is susceptible to biotic or abiotic degradation. This review identified six transformation products that have been detected in soil at concentrations greater than 5 mg kg^{-1}: carbofuran, 2-hydroxy-4-chlorobenzoic acid, 2,4-dichlorobenzoic acid, p,p'-DDD, o,p'-DDD, and p,p'-DDE. The three DDT transformation products were detected in soil from a former cattle tick dip site in Australia (Van Zweiten et al. 2001). Therefore, these concentrations can be considered an exception rather than the rule because sampling was targeted to a known hotspot. Similarly, high concentrations of the chlorfenvinphos transformation products, 2-hydroxy-4-chlorobenzoic acid (5.7 mg kg^{-1}) and 2,4-dichlorobenzoic acid (7.9 mg kg^{-1}) in soil were detected following a targeted sampling strategy (reported in PSD 1994c). Chlorfenvinphos was applied around the stem of cauliflower and brussel sprout plants, with subsequent soil samples collected 10cm around the base of the plants again targeting the sampling to known hotspots, which may not be representative of the field as a whole. The final transformation product identified was the active component of the insecticide benfuracarb, carbofuran (6.3 mg kg^{-1}) (PSD 1988a). This pro-pesticide utilizes the degradation of benfuracarb to form the potent acetylchloinesterase inhibitor carbofuran and, in soil, undergoes

hydrolysis to carbofuran (Roberts and Hutson 1999), so high concentrations can be expected.

2.6.2 Surface water

Whether transformation products are present in surface waters at higher or lower levels than the parent compound depends on the pesticide and transformation products concerned. Seven transformation products have been identified in tile drain water (Appendix A, Table A4). Four of these have been observed at peak concentrations greater than 3 $\mu g\ L^{-1}$: cyanazine amide, DEA, metolachlor OA and metolachlor ESA. Following the agricultural application of atrazine and cyprazine, the peak concentrations observed in tile drains were larger for the parent compounds for two consecutive seasons than for the transformation product DEA. However, the total loss over the same period was greater for DEA than for either herbicide. Total losses via tile drains of two cyanazine transformation products (cyanazine amide and DIA) are an order of magnitude greater than the parent compound, loses of DIA formed solely from atrazine are an order of magnitude less than the parent compound (Muir and Baker 1976). Metolachlor transformation products (metolachlor ESA and metolachlor OA) were detected in tile drain samples at concentrations at least two orders of magnitude greater than their herbicidal parent (Phillips et al. 1999).

A study of streams in the Midwestern US monitored for triazine and chloroacetamide herbicides and their transformation products (Kalkhoff et al. 2003). The transformation products monitored for were the ESA and OA of alachlor, acetochlor, and metolachlor and the triazine transformation products cyanazine amide, DEA, DIA, and HA. The frequency of detection for individual transformation products in 70 streams varied from 23 to 96%, with seven transformation products detected in more than 50% of the samples. Multiple transformation products were detected in all samples analyzed (Kalkhoff et al. 2003). In a study of streams and rivers of Northern Missouri and Southern Iowa, DEA, DIA, HA, atrazine, and cyanazine amide were detected in > 95% of the

samples (Lerch and Blanchard 2003). In surface water, the two main metolachlor transformation products, ESA and OA, were the major residue of metolachlor present (Phillips et al. 1999).

If these surface waters are to be used for drinking water supply, it is important to determine in which phase the contaminants are found. In one study no atrazine and alachlor transformation products were detected in suspended sediment in the Mississippi River and its tributaries, while both parents and their transformation products were detected in the dissolved phase (Pereira and Rostad 1990). This is important in determining which processes will be the most effective in removing these compounds during water treatment. Treatment methods that use sorption, e.g. granular activated carbon and power activated carbon, maybe most effective for transformation products in the dissolved phase, while filtration methods, e.g. rapid gravity sand filters, maybe better for removing transformation products that are sorbed to suspended sediment.

Ultimately when transformation products are present in rivers and streams, they will be transported to estuarine and marine environments. The annual load of atrazine discharge to the Gulf of Mexico in 1993 was estimated at 642 t (Clark et al. 1999). These calculations did not take into account the discharge of atrazine transformation products which could drastically increase the total atrazine residue. The estimated discharge of DEA into the Greek Amvrakikos Gulf is greater than atrazine, 127.5g day^{-1} and 122.7g day^{-1}, respectively (Albanis and Hela 1998).

2.6.3 Groundwater

Transformation products have been detected in groundwater at higher concentrations (Albanis et al. 1998; Ferrer et al. 2000) and more frequently (Kolpin et al. 2000; Kolpin et al. 2001) than their parental compounds. A number of transformation products have been identified in groundwater during monitoring studies (Appendix A, Table A4). Primarily it is the transformation

products of the triazines, i.e. atrazine, cyanazine and simazine, and the chloroacetamides, i.e. alachlor, acetochlor and metolachlor, that have been detected in groundwater. Twenty-four transformation products observed in groundwater originate from these six herbicides while monitoring data concerning transformation products from other pesticide chemical groups are limited. The presence of transformation products in groundwater depends on the aquifer type, well depth, surrounding geography, time of sampling, i.e. pre or post application, extent of pesticide usage, transformation product formation, mobility, and persistence (Burkart and Kolpin 1993; Kolpin et al. 1996a; Blanchard and Donald 1997; Kolpin et al. 1997). The peak water concentration for transformation products identified in this review was 158.2 $\mu g\ L^{-1}$ from the combined concentration of dacthal diacid and dacthal monoacid in a groundwater sample collected from the Malheur River Basin, Oregon (Monohan et al. 1995).

As well as the vertical movement of vadose zone water, the transport of transformation products to groundwater has been attributed to the hydraulic connection of groundwater to surface waters such as rivers. The movement of transformation products from rivers, through aquifers and into collector wells, driven by the abstraction of water has been identified as a means for pesticides and their transformation products to enter drinking waters (Verstraeten et al. 1999). Once transformation products have entered groundwater, their subsequent movement can be more, e.g. DIA, and less, e.g. DEA, retarded when compared to their parents, e.g. atrazine (Widmer and Spalding 1995).

During comprehensive monitoring programs of pesticides and their transformation products in groundwater, transformation products are some of the most frequently detected compounds (Kolpin et al. 1996b; Kolpin et al. 1997; Kolpin et al. 1998; Kolpin et al. 2000). Moreover, p,p'-DDE, a transformation product of the insecticide DDT, is still being detected in groundwater decades after a ban on the use parent compound was imposed (Kolpin et al. 1996b). The detection frequency of individual herbicides in groundwater is increased considerably when their transformation products are considered (Kolpin et al.

1998). Moreover, for a number of herbicides, the majority of the total herbicide concentration was in the form of transformation products (Kolpin et al. 2000; Kolpin et al. 2001). Therefore, to fully establish the effect pesticide use has on groundwater, it is necessary to quantify the transformation products present. Generally, when groundwater monitoring for transformation products is undertaken, it is a few primary transformation products that are actively sought for each pesticide. However, a range of additional transformation products present in low concentrations will also be present in the groundwater.

2.7 Occurrence and Fate in Drinking Water

Pesticide transformation products have been regularly identified in groundwater and surface waters (Table 5; Appendix A, Table A4). Hence, transformation products must be present in raw water abstracted from these sources. There is therefore, the potential for these transformation products to be present in finished drinking water if they are not removed during the treatment process. Table 6 provides a summary of transformation product occurrence data in raw and finished drinking waters. Five OP insecticide transformation products have been identified in water-supply reservoirs. Azinphos-methyl oxon, the active form of the pesticide azinphos-methyl has been monitored at a mean concentration of 0.26 $\mu g\ L^{-1}$ in the raw water for eleven drinking water treatment plants in the US (Nguyen et al. 2004). Moreover, the three most commonly identified atrazine transformation products, DEA, DIA, and HA have been measured at 0.38, 0.14 and 0.8 $\mu g\ L^{-1}$ respectively in reservoirs (Solomon et al. 1996). DDA is a polar transformation product of the organochlorine insecticide DDT, the use of which has been banned for a number of decades. However, in Germany, several drinking water wells have been closed to keep the DDA concentrations below the 0.1 $\mu g\ L^{-1}$ drinking water tolerance level set by the EU (Heberer and Dünnbier 1999).

Table 6. Summary of maximum concentrations of transformation products in raw and finished drinking waters

Transformation product	Parent pesticide [a]	Concentration	Limit of detection	Country	Reference
Raw source water					
hydroxyacetochlor	acetochlor	198 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
deschloroacetochlor	acetochlor	35 ng L^{-1} [b]	0.07 ng L^{-1}	USA	Hladik et al. 2006
acetochlor oxanilic acid	acetochlor	1170 ng L^{-1} [b]	7 ng L^{-1}	USA	Hladik et al. 2006
acetochlor ethane sulfonic acid	acetochlor	1080 ng L^{-1} [b]	100 ng L^{-1}	USA	Hladik et al. 2006
2-chloro-2'-ethyl-6'-methylacetanilide	acetochlor	167 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
2-hydroxy-2'-ethyl-6'-methylacetanilide	acetochlor	105 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
2-ethyl-6-methylaniline	acetochlor	<25 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
2'-ethyl-6'-methylacetanilide	acetochlor	57 ng L^{-1} [b]	8 ng L^{-1}	USA	Hladik et al. 2006
hydroxyalachlor	alachlor	43 ng L^{-1} [b]	3 ng L^{-1}	USA	Hladik et al. 2006
deschloroalachlor	alachlor	14 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
2-chloro-2'-6'-diethylacetanilide	alachlor	15 ng L^{-1} [b]	0.1 ng L^{-1}	USA	Hladik et al. 2006
2-hydroxy-2'-6'-diethylacetanilide	alachlor	104 ng L^{-1} [b]	0.7 ng L^{-1}	USA	Hladik et al. 2006
2-hydroxy-2'-6'-diethyl-N-methylacetanilide	alachlor	1.7 ng L^{-1} [b]	4 ng L^{-1}	USA	Hladik et al. 2006
2'-6'-diethylacetanilide	alachlor	43 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
2,6-diethylaniline	alachlor	<11 ng L^{-1} [b]	10 ng L^{-1}	USA	Hladik et al. 2006
alachlor oxanilic acid	alachlor	216 ng L^{-1} [b]	7 ng L^{-1}	USA	Hladik et al. 2006
alachlor ethane sulfonic acid	alachlor	945 ng L^{-1} [b]	100 ng L^{-1}	USA	Hladik et al. 2006
deethylatrazine	atrazine	0.682 µg L^{-1} [b]	-	USA	Coupe and Blomquist 2004
deethylatrazine continued	atrazine	594 ng L^{-1} [b]	0.3 ng L^{-1}	USA	Hladik et al. 2006
deisopropylatrazine	atrazine	199 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
hydroxyatrazine	atrazine	0.8 µg L^{-1} [c]	-	USA	Solomon et al. 1996
azinphos-methyl-oxon	azinphos-methyl	0.263 µg L^{-1} [c]	0.031 µg L^{-1}	USA	Nguyen et al. 2004
o-p'-DDA	DDT	0.28 µg L^{-1}	-	Germany	Heberer and Dünnbier 1999
p-p'-DDA	DDT	1.7 µg L^{-1}	-	Germany	Heberer and Dünnbier 1999
deschlorodimethenamid	dimethenamid	14 ng L^{-1} [b]	0.1 ng L^{-1}	USA	Hladik et al. 2006
disulfoton sulfone	disulfoton	0.013 µ g L^{-1} [c]	0.005 µg L^{-1}	USA	Nguyen et al. 2004
disulfoton sulfoxide	disulfoton	0.06 µg L^{-1} [c]	0.016 µg L^{-1}	USA	Nguyen et al. 2004
fenamiphos sulfone	fenamiphos	0.005 µg L^{-1} [c]	0.008 µg L^{-1}	USA	Nguyen et al. 2004
fenamiphos sulfoxide	fenamiphos	0.021 µg L^{-1} [c]	0.008 µg L^{-1}	USA	Nguyen et al. 2004
malaoxon	malathion	ND	0.005 µg L^{-1}	USA	Nguyen et al. 2004
hydroxymetolachlor	metolachlor	217 ng L^{-1} [b]	1 ng L^{-1}	USA	Hladik et al. 2006
deschlorometolachlor	metolachlor	32 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
metolachlor morpholinone	metolachlor	63 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
metolachlor propanol	metolachlor	208 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
deschloroacetylmetachlor	metolachlor	39 ng L^{-1} [b]	0.1 ng L^{-1}	USA	Hladik et al. 2006
deschloroacetyl metachlor propanol	metolachlor	17 ng L^{-1} [b]	0.8 ng L^{-1}	USA	Hladik et al. 2006
metachlor oxanilic acid	metolachlor	687 ng L^{-1} [b]	7 ng L^{-1}	USA	Hladik et al. 2006
metachlor ethane sulfonic acid	metolachlor	1580 ng L^{-1} [b]	90 ng L^{-1}	USA	Hladik et al. 2006

Table 6. Summary of maximum concentrations of transformation products in raw and finished drinking waters

Transformation product	Parent pesticide [a]	Concentration	Limit of detection	Country	Reference
Finished drinking water					
hydroxyacetochlor	acetochlor	64 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
deschloroacetochlor	acetochlor	31 ng L^{-1} [b]	0.07 ng L^{-1}	USA	Hladik et al. 2006
acetochlor oxanilic acid	acetochlor	551 ng L^{-1} [b]	7 ng L^{-1}	USA	Hladik et al. 2006
acetochlor ethane sulfonic acid	acetochlor	845 ng L^{-1} [b]	100 ng L^{-1}	USA	Hladik et al. 2006
2-chloro-2'-ethyl-6'-methylacetanilide	acetochlor	163 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
2-hydroxy-2'-ethyl-6'-methylacetanilide	acetochlor	67 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
2-ethyl-6-methylaniline	acetochlor	<25 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
2'-ethyl-6'-methylacetanilide	acetochlor	57 ng L^{-1} [b]	8 ng L^{-1}	USA	Hladik et al. 2006
hydroxyalachlor	alachlor	34 ng L^{-1} [b]	3 ng L^{-1}	USA	Hladik et al. 2006
deschloroalachlor	alachlor	0.7 ng L^{-1} [b]	-	USA	Hladik et al. 2006
2-chloro-2'-6'-diethylacetanilide	alachlor	11 ng L^{-1} [b]	0.1 ng L^{-1}	USA	Hladik et al. 2006
2-hydroxy-2'-6'-diethylacetanilide	alachlor	85 ng L^{-1} [b]	0.7 ng L^{-1}	USA	Hladik et al. 2006
2-hydroxy-2'-6'-diethyl-N-methylacetanilide	alachlor	1.7 ng L^{-1} [b]	4 ng L^{-1}	USA	Hladik et al. 2006
2'-6'-diethylacetanilide	alachlor	38 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
2,6-diethylaniline	alachlor	<11 ng L^{-1} [b]	10 ng L^{-1}	USA	Hladik et al. 2006
alachlor oxanilic acid	alachlor	136 ng L^{-1} [b]	7 ng L^{-1}	USA	Hladik et al. 2006
alachlor ethane sulfonic acid	alachlor	743 ng L^{-1} [b]	100 ng L^{-1}	USA	Hladik et al. 2006
deethylatrazine	atrazine	0.352 µg L^{-1} [b]	-	USA	Coupe and Blomquist 2004
deisopropylatrazine	atrazine	75 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
azinphos-methyl-oxon	azinphos-methyl	0.026 µg L^{-1} [c]	0.031 µg L^{-1}	USA	Nguyen et al. 2004
deschlorodimethenamid	dimethenamid	25 ng L^{-1} [b]	0.1 ng L^{-1}	USA	Hladik et al. 2006
disulfoton sulfone	disulfoton	ND	0.005 µg L^{-1}	USA	Nguyen et al. 2004
disulfoton sulfoxide	disulfoton	ND	0.016 µg L^{-1}	USA	Nguyen et al. 2004
fenamiphos sulfone	fenamiphos	0.011 µg L^{-1} [c]	0.008 µg L^{-1}	USA	Nguyen et al. 2004
fenamiphos sulfoxide	fenamiphos	0.022 µg L^{-1} [c]	0.008 µg L^{-1}	USA	Nguyen et al. 2004
malaoxon	malathion	0.106 µg L^{-1} [c]	0.005 µg L^{-1}	USA	Nguyen et al. 2004
hydroxymetolachlor	metolachlor	61 ng L^{-1} [b]	1 ng L^{-1}	USA	Hladik et al. 2006
deschlorometolachlor	metolachlor	30 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
metolachlor morpholinone	metolachlor	37 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
metolachlor propanol	metolachlor	73 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
deschloroacetylmetachlor	metolachlor	35 ng L^{-1} [b]	0.1 ng L^{-1}	USA	Hladik et al. 2006
deschloroacetyl metachlor propanol	metolachlor	22 ng L^{-1} [b]	0.8 ng L^{-1}	USA	Hladik et al. 2006
metachlor oxanilic acid	metolachlor	215 ng L^{-1} [b]	7 ng L^{-1}	USA	Hladik et al. 2006
metachlor ethane sulfonic acid	metolachlor	1530 ng L^{-1} [b]	90 ng L^{-1}	USA	Hladik et al. 2006

a - pesticide identified in the reference as the source of the transformation product

b - peak concentration during study

c - median or mean concentration

Two areas of importance concerning the fate of pesticide transformation products during drinking water treatment are, their removal from raw water; and their possible transformation during treatment. Treatment processes such as coagulation, flocculation, sedimentation, and membrane filtration will assist in the removal of transformation products associated with suspended sediment in the raw water. Activated carbon adsorption, reverse osmosis, and nanofiltration can assist in the removal of transformation products associated with the aqueous phase (Wang and Song 2004), there is the potential for disinfection processes used during water treatment such as oxidation and advanced oxidation utilizing, ozone, hydrogen peroxide, and UV to transform organic compounds present in the raw water to additional compounds that need to be considered (EPA 2001a).

It is the presence and transformation of both pesticides and their environmental transformation products to additional water treatment transformation products that could pose a risk to human health. There is very limited data available in the literature identifying which degradation pathways pesticides and their environmental transformation products would undergo during water treatment. There are a number of processes utilized during water treatment that remove pesticides and their transformation products, however, chemical treatments can transform pesticides and their transformation products into additional compounds (EPA 2001a).

Data are available on the removal of pesticides from raw water by various water treatment processes, such as advanced oxidation with ozone and UV radiation (Collivignarelli and Sorlini 2004), nanofiltration (Van der Bruggen et al. 2001) and granular activated carbon (Feleke and Sakakibara 2001). Generally, pesticide transformation products are smaller and more polar than the parent compounds which could decrease the removal efficiency during treatment processes. However, only limited data are available on water treatment process removal efficiencies of pesticide environmental transformation products.

The oxidative desulphorisation of organophosphorus insecticides occurs during chlorination when the pesticides are present in raw water. This is where the thiophosphate moiety (P=S) is transformed to a P=O moiety (Zhang and Pehkonen 1999). This is an important transformation, especially for human health, because it is the oxon form that is the active component of the pesticide. These transformation products are very potent acetylcholinesterase inhibitors, a mode of action that can affect humans (Giesy et al. 1999). During the monitoring of supply reservoirs in the USA, the oxon transformation product of malathion, malaoxon, was not detected in the raw water, while the parent compound was detected at 0.032 $\mu g\ L^{-1}$. Following water treatment, malathion was not detected in the finished drinking water but maloxon was detected at 0.106 $\mu g\ L^{-1}$ (Nguyen et al. 2004). These oxon transformation products of OP insecticides, such as diazoxon, are stable in water after their formation even following chlorination. The carbamate insecticide thiobencarb and its transformation products formed following chlorination are degraded completely within 2 hours by the presence of chlorine in the water (Magara et al. 1994). Therefore depending on the pesticide in question, the chlorination process can both transform insecticides to stable active transformation products and rapidly degrade them and their transformation products. The herbicide isoxaflutole rapidly degrades to a stable phytotoxic transformation product, diketonitrile, under environmental conditions. Chlorination of water containing diketonitrile rapidly degrades this compound to a nonbiologically active benzoic acid transformation product (Lin et al. 2003).

Using ozonation as a disinfection process instead of chlorination can also transform organic compounds present in the raw water. DEA, DIA, deisopropylatrazine amide, and 2-chloro-4,6-diamino-s-triazine have been identified as transformation products formed from the major degradation pathway following the ozonation of water containing atrazine (Adams and Randtke 1992). When atrazine undergoes advanced oxidation during the water treatment process, two transformation products, not observed during environmental degradation, are formed, 2-chloro-4-ethylimino-6-

isopropylamino-s-triazine and 6-amino-2-chloro-4-ethylimino-s-triaizne (Acero et al. 2000).

Two transformation products of the insecticide aldicarb, aldicarb sulfoxide and aldicarb sulfone, can be removed during water treatment by reverse osmosis. The efficiency of removal of these compounds depends on the membrane composition used. However, when these transformation products are present in raw water (groundwater) in the 11-47 $\mu g\ L^{-1}$ concentration range, removal efficiency is in excess of 90% (reported in EPA 2001a).

2.7.1 Drinking Water Standards

The EPA has set maximum contaminant levels (MCL) for three individual pesticide transformation products, heptachlor epoxide, aldicarb sufone and aldicarb sulfoxide (Table 7). An MCL of 7 $\mu g\ L^{-1}$ has been set for a combined concentration of aldicarb and its two transformation products (EPA 2004a). Current drinking water standards for pesticides in the EU are governed by the Drinking Water Directive (98/83/EC). There are no discrete pesticide or pesticide transformation product drinking water quality standards set in the EU, however, concentrations of any individual pesticide and its "relevant metabolites" must not exceed 0.1 $\mu g\ L^{-1}$, with a total pesticide concentration not exceeding 0.5 $\mu g\ L^{-1}$ (European Commission 1998). In Australia, the maximum acceptable concentration (MAC) for atrazine is set at 40 $\mu g\ L^{-1}$. This concentration is set on the basis that DEA, DIA, diaminochlorotriazine and HA may constitute approximately 50% of the total atrazine-derived triazine compounds in environmental waters (NHMRC 1996). Currently the health based guidelines for drinking water set by the World Health Organisation contain drinking water standards for pesticides. There is a combined pesticide and transformation product guideline for DDT of 1 $\mu g\ L^{-1}$ (WHO 2004).

Table 7. Drinking water standards set for pesticide transformation products

Region	Compound	Parent pesticide	Standard ($\mu g\ L^{-1}$)	Source
Australia	heptachlor and heptachlor epoxide		0.05 [b]	NHMRC 1996
Canada	2,3,4,6-tretrachlorophenol	pentachlorophenol	100 [c]	Health Canada 1987
Canada	2,4,6-trichlorophenol	pentachlorophenol	5 [c]	Health Canada 1987
Canada	2,4-dichlorophenol	phenoxycarboxylic acid herbicides	900 [c]	Health Canada 1987
Canada	aldicarb, aldicarb sulfone and aldicarb sulfoxide		9 [c]	Health Canada 1995
Canada	atrazine and N-dealkylated metabolites		5 [c]	Health Canada 1993
Canada (Ontario)	DDT and metabolites		30	OCWA 2002
Canada (Ontario)	heptachlor and heptachlor epoxide		3	OCWA 2002
Canada (Ontario)	total lindane		4	OCWA 2002
EU	pesticides and their relevant metabolites		0.1	European Commission 1998
EU	total pesticides		0.5	European Commission 1998
USA	aldicarb sulfone	aldicarb	3 [a]	EPA 2004a
USA	aldicarb sulfoxide	albicarb	4 [a]	EPA 2004a
USA	aldicarb, aldicarb sulfone and aldicarb sulfoxide		7 [a]	EPA 2004a
USA	heptachlor epoxide	heptachlor	0.2 [a]	EPA 2004a
World	DDT and metabolites		1 [b]	WHO 2004

a - maximum contaminate level (MCL)

b - guidance level

c - maximum acceptable concentration (MAC)

3 Estimation of the Properties of Transformation Products

3.1 Introduction

An extensive range of transformation products have been identified during the examination of biotic and abiotic degradation of pesticides and other synthetic chemicals (Roberts 1998; Roberts and Hutson 1999; Aizawa 2001). A number of transformation products may be formed from any one compound and whilst physico-chemical property information maybe determined for the most prevalent, it would be beneficial if validated techniques were available to allow the information to be ascertained for all.

Current EU guidance suggests that data requirements for pesticide transformation products, determined during the generation of a dossier for the parent pesticide, do not have to be addressed solely by experimental studies (European Commission 2002a). Physico-chemical properties and environmental parameters required for risk assessment are currently determined experimentally for relevant transformation products but not for more minor compounds (European Commission 1994). Whilst the determination for minor or non-relevant compounds is not required for pesticide registration, these would be useful data to acquire for the application of screening and prioritisation methodologies (Gustafson 1989; Sinclair et al. 2006). Such approaches can be used to focus analytical monitoring towards compounds of concern and adjust treatment methods to ensure they are removed from finished drinking waters. Predictive approaches could be utilised to provide physico-chemical and environmental properties for transformation products during prioritisation, ranking and/or priority setting activities (Russom et al. 2003).

Recently concern has been expressed over the potential for the production of harmful by-products from pesticide transformation products formed during drinking water treatments employed to waters prior to distribution to consumers

(European Commission 2007). Processes such as chlorination can activate pro-insecticides to transformation products with specific modes of action to which humans are susceptible, e.g. acetylcholine esterase inhibition (Magara et al. 1994; Zhang and Pehkonen 1999). In order to screen or identify compounds of concern there is a requirement to determine those which may contaminate source drinking waters, identify the by-products that maybe formed and determine those compounds that may pose a hazard to human health. The accurate determination of physico-chemical properties, such as vapour pressure and octanol-water partition coefficient, and environmental parameters, such as rate of degradation and sorption behaviour in soils, would be critical to modelling and prioritisation techniques employed to determine the risks posed to ecosystems and/or consumers.

The range of quantitative structure property relationships (QSPR) available either within the literature, integrated into freely available or propriety software or available via the web, is vast. The predictive domain of these approaches is determined by the chemicals used to develop the relationship. Approaches are available that can provide a physico-chemical property for estimates for specific chemical classes or a diverse range of compounds. Whilst the suitability and accuracy of some approaches have been examined for various properties, e.g. acid dissociation constant (Hilal and Karickhoff 1995), vapour pressure (Dearden 2003) and soil sorption (Dearden 2004), little work has been conducted to confirm whether these approaches are suitable for providing property predictions specifically for pesticide transformation products. Therefore the aim of this study was to explore the use of predictive techniques for estimating key environmental and physico-chemical properties for pesticide transformation products necessary to implement priority approaches. A pesticide and transformation product experimental property dataset was collated and briefly compared. The dataset was then used to statistically evaluate a variety of QSPR approaches suitable for estimating, octanol-water partition coefficient (K_{ow}), acid dissociation constant (pKa), vapour pressure, henry's law constant, organic carbon partition coefficient (K_{oc}) and soil persistence (DT_{50}/t½).

3.2 Material and Methods

3.2.1 Collation and comparison of transformation product and pesticide datasets

Environmental pesticide transformation products were identified using degradation route compendiums (Roberts 1998; Roberts and Hutson 1999; Aizawa 2001), regulatory review documents (EPA 2005; PSD 2005; PMRA 2005; European Commission 2005; APVMA 2005) and the publicly available literature. Only those transformation products produced from biotic and abiotic degradation in the environment were considered. For each of the transformation products and pesticides identified, physico-chemical property and environmental property data were collected from KOW, PHYSPROP and EFDB databases (SRC 2005a; SRC 2005b; SRC 2005c), The Pesticide Manual (Tomlin 2000), degradation route compendiums (Roberts 1998; Roberts and Hutson 1999), the report of Belfroid et al. (1996) and regulatory review documents (EPA 2005; PSD 2005; PMRA 2005; European Commission 2005).

A comparison between parent pesticide and transformation product physico-chemical properties was undertaken to establish whether any general principles could be ascertained. Where possible a direct comparison was undertaken for properties such as K_{ow} and water solubility which are represented by single data points and allow a direct comparison. In order to increase the number of comparative data points for the analysis of vapour pressure, pesticide and transformation product data were compared if the temperature reported during the experimental derivation was within 5°C. A comparison of dissociation data was more complicated since within the literature if no dissociation data are available for transformation products then it is impossible to determine whether this is because they do not dissociate or no experimental data are available. For pesticides there is no uncertainty since information is readily abundant. Therefore transformation products that had collated dissociation data were

compared to data for their respective parent compounds, no comparison was undertaken to examine the relationships that exist between transformation products that do not dissociate and their parent pesticides. (*For an equivalent comparison of environmental properties, adsorption and soil persistence, see Chapter 2*).

3.2.2 Property estimation

A number of predictive approaches were chosen for evaluation that provide the user with estimates of physico-chemical and environmental properties for pesticides and transformation products. Approach selection was dependent on their ease of use, availability and appropriateness for agrochemicals. The selected approaches either operated via a software or web-based front-end or were simple linear relationships. Approaches were not selected for evaluation that required complicated property/structural molecular descriptors as suitable programs were not available to generate these input parameters. The predictive approaches considered are provided in Table 8.

All the single linear relationships chosen use an alternative physico-chemical property from which to estimate the property of interest, therefore data collated to evaluate methods that estimate the required property were used for this purpose. Linear relationships were therefore constrained by the availability of experimentally determined input data, approaches that require structural entry for estimation were not constrained by such an extent.

Table 8. The predictive approaches evaluated during this study

Property	Method (version)	Data Input[a]	Availability/Relationship	Reference
K_{oc}	PCKOCWIN (1.66)	SMILES notation	Free software	Meylan and Howard 1995; EPA 2004b
	ASTER [c]	SMILES notation	Limited access software	Russom et al. 1991
	Briggs 1981	Log K_{ow}	Log K_{oc} = 0.52 log K_{ow} + 1.12	Briggs 1981
	Hodson and Williams 1988	Log K_{ow}	Log K_{oc} = 0.827log K_{ow} + 0.293	Hodson and Williams 1988
	Kanazawa 1989	Log K_{ow}	Log K_{oc} = 0.402 log K_{ow} + 1.071	Kanazawa 1989
	Kenaga and Goring 1980	Log K_{ow}	Log K_{oc} = 0.544 log K_{ow} + 1.377	Kenaga and Goring 1980
	Lyman et al. 1990	Log K_{ow}	Log K_{oc} = 1.029 log K_{ow} - 0.18	Lyman et al. 1990
	Sabljić et al. 1995	Log K_{ow}	Log K_{oc} = 0.47 log K_{ow} + 1.09	Sabljic et al. 1995
	Seth et al. 1999	Log K_{ow}	Log K_{oc} = 1.03 log K_{ow} - 0.61	Seth et al. 1999
	Briggs 1981 (WS)	Log S (S in ppm)	Log K_{oc} = -0.356 log S + 3.01	Briggs 1981
	Kenaga and Goring 1980 (WS)	Log S (S in mg/L)	Log K_{oc} = -0.55 log S + 3.64	Kenaga and Goring 1980
K_{ow}	KOWWIN (1.67)	SMILES notation	Free software	Meylan and Howard 1995; EPA 2004b
	ClogP (4.82)	SMILES notation	Web based	Daylight Chemical Information Systems 2004
	LogP	SMILES notation	Web based	Interactive Analysis 2004
	AlogPS (2.1)	SMILES notation	Web based	Tetko et al. 2001b; Tetko and Tanchuk 2002; Virtual Computational Chemistry Laboratory 2004
	miLogP [b]	SMILES notation	Web based	Molinspiration Cheminformatics 2004
	XLogP (2.0) [b]	SMILES notation	Web based	Wang et al. 1997; Institute of Physical Chemistry 2004
Henry's Law constant	HENRYWIN (1.90)	SMILES notation	Free software	Meylan and Howard 1991; EPA 2004b
	ASTER [c]	SMILES notation	Limited access software	Russom et al. 1991
Vapour pressure	MPBPWIN (1.41)	SMILES notation	Free software	EPA 2004b
	ASTER [c]	SMILES notation	Limited access software	Russom et al. 1991
Water solubility	WSKOWWIN (1.41)	SMILES notation	Free software	Meylan et al. 1996; EPA 2004b
	AlogPS (2.1)	SMILES notation	Web based	Tetko et al. 2001a; Virtual Computational Chemistry Laboratory 2004
	LogS [b]	SMILES notation	Web based	Virtual Computational Chemistry Laboratory 2004
	ASTER [c]	SMILES notation	Limited access software	Russom et al. 1991
Soil degradation	BIOWIN (4.02)	SMILES notation	Free software	Howard et al. 1992; Boethling et al. 1994; EPA 2004b
	PBT profiler	SMILES notation	Web based	EPA 2004c

[a] - data input maybe possible by other means, e.g. CAS Number, SMILES or 2D chemical structure, but this was the method used to generate predictions during the study

[b] - predictions made through the Virtual Computational Chemistry Laboratory website [Virtual Computational Chemistry Laboratory 2004]

[c] - predictions provided by the US Environmental Protection Agency after supplying the transformation product and pesticide SMILES notation in .txt file format

The software or web-based front end approaches examined require chemical structure as the input. This is usually in the form of Simplified Molecular Input Line Entry System (SMILES) notation (Weininger 1988). Pesticide SMILES notation were obtained by using the CAS/SMILES database present in

KOWWIN version 1.67 (EPA). CAS numbers for pesticides were obtained from The Pesticide Manual (Tomlin 2000). Transformation product SMILES notation were derived from their two-dimensional structure identified within degradation compendiums and regulatory review documents. Two-dimensional transformation product structures were saved as .cdx files in ChemDraw version 8.0 (CambridgeSoft Corporation). Structures were either drawn manually, downloaded from the website Chemfinder.com (CambridgeSoft Corporation) or when the structure was solely provided as an IUPAC name, then the structure was generated using the ChemDraw add-on NamExpert version 6.0 (ChemInnovation Software). SMILES notation were then generated using the 'convert to SMILES' function in Accord for Excel version 5.0 (Accelrys Inc.), an Excel 2000 version 9.0 (Microsoft Corporation) add-on.

3.2.3 Statistical Analysis

The approaches were evaluated using a revised version of the methodology proposed by Moore et al. (2003), i.e. the best performing approach is identified by ranking the approaches based on selected individual summary statistics and then determining an overall rank. However the ordinal ranking system was replaced by a ranking system that provided a measure of the ability of a technique within each of the chosen statistics. The techniques were ranked on their distance from the optimum summary statistic value standardized using the maximum distance from the optimum for all the techniques tested. An overall score was obtained by then calculating the mean of the individual rank scores, the best performing technique was identified as the one with a mean rank score nearest to zero, i.e. perfect performance. Genstat version 7.2 (VSN International) and Excel version 9.0 (Microsoft Corporation) were used to analyse the data. The statistics generated for each technique are detailed below; the summary statistics used for ranking are identified with an asterisk (*).

- actual number of compounds a technique could provide a prediction for*
- percentage positive deviation*

- mean absolute deviation*
- maximum absolute deviation
- minimum absolute deviation
- mean squared absolute deviation*
- % of compounds > 1 order of magnitude from experimental value*
- % of compounds > 2 orders of magnitude from experimental value
- % of compounds > 3 orders of magnitude from experimental value
- pearson correlation coefficient*
- slope
- intercept

The percentage positive deviation is the percentage of predictions that were over or under estimated from perfect correlation. If a predictive technique does not have a tendency to over or under predict values, i.e. over predicts as many values as it under predicts then you would expect the percentage positive deviation to be 50%. Therefore this statistic is used as a measure of the tendency of a package to over or under predict. The data reported for this statistic is the distance from 50%, i.e. if positive the technique has a tendency to under predict the data, if negative the technique has a tendency to over predict the data, whilst the further away from zero the more exaggerated this tendency. A one sample binomial test was used to identify whether the tendency was significant at the 95% confidence limit. Statistics were chosen to quantify different prediction capabilities. The Pearson correlation coefficient was chosen instead of the slope of correlation because it would be less influenced by a few large outliers. Mean absolute deviation and mean squared absolute deviation where chosen to provide a measure of the extent of 'scatter'.

For each approach two analyses were undertaken, the ability to provide data for 'all' chemicals with experimentally derived test data and the ability to provide data for chemicals 'common' to all the predictive approaches for that end-point, i.e. the set of compounds that all approaches evaluated could provide a

prediction for. An evaluation of 'all' compounds includes a measure of the ability of a specific approach to provide an estimate for a query molecule, whilst an evaluation of 'common' compounds provides a fairer means by which to interpret the accuracy between approaches. Where a number of approaches where identified as performing well, then an examination of whether predictive ability could be increased for the transformation product dataset by combining the best performing approaches was undertaken.

3.3 Results and Discussion

3.3.1 Collated Dataset

Table 9 provides a summary of the available transformation product and pesticide data that was considered suitable for evaluating the selected predictive approaches, information on the extent of pesticide class coverage within the dataset is also provided. The analytical dataset for environmental transformation products comprised 320 compounds from 125 pesticide parent compounds, whilst the pesticide dataset comprised 476 pesticides from 61 chemical classes.

Table 9. Summary of the data availability for transformation product and pesticide analytical datasets

Data type	Transformation product data	Pesticide data
Physico-chemical properties		
Henry's law constant	50	61
K_{ow}	160	445
pKa	91	442[b]
Vapour pressure	93	410
Water solubility	139	463
Environmental properties		
K_{oc}	115	300
Soil $DT_{50}/t_{½}$	85	-
Dataset composition		
Number of compounds	320	476
Herbicides	64[a]	174
Fungicides	25[a]	103
Insecticides	28[a]	155
Other	8[a]	44
Chemical classes	47[a]	61

[a] - data for parental pesticides
[b] - includes pKa data where pesticides were reported not to dissociate

3.3.2 Pesticide and Transformation Product Property Comparison

Overall pesticide transformation products were more hydrophilic (81.1%), more water soluble (88.6%) and more volatile (91.2% for vapour pressure and 71.4% for henry's law constant) than their respective parental pesticides (Figure 10). It is inevitable that transformation products exhibit properties different to their parents since there has been slight and/or extensive structural change and they are not subjected to the extensive selection pressures placed on pesticides during their development. Whilst high volatility is a desirable trait for some classes of pesticides, e.g. fumigants and soil sterilants, most pesticides could not perform the desired task if, once applied they where lost to the atmosphere. Transformation products are generally more volatile with 71.7% exhibiting a vapour pressure of more than two orders of magnitude more than their pesticides. When soil sterilants and fumigants were removed from the comparison, the remaining transformation products from pesticides with a vapour pressure greater than 0.01 Pa were all more volatile than their respective parent pesticides. Moreover, only three transformation products exhibited a decrease in volatility by more than an order of magnitude.

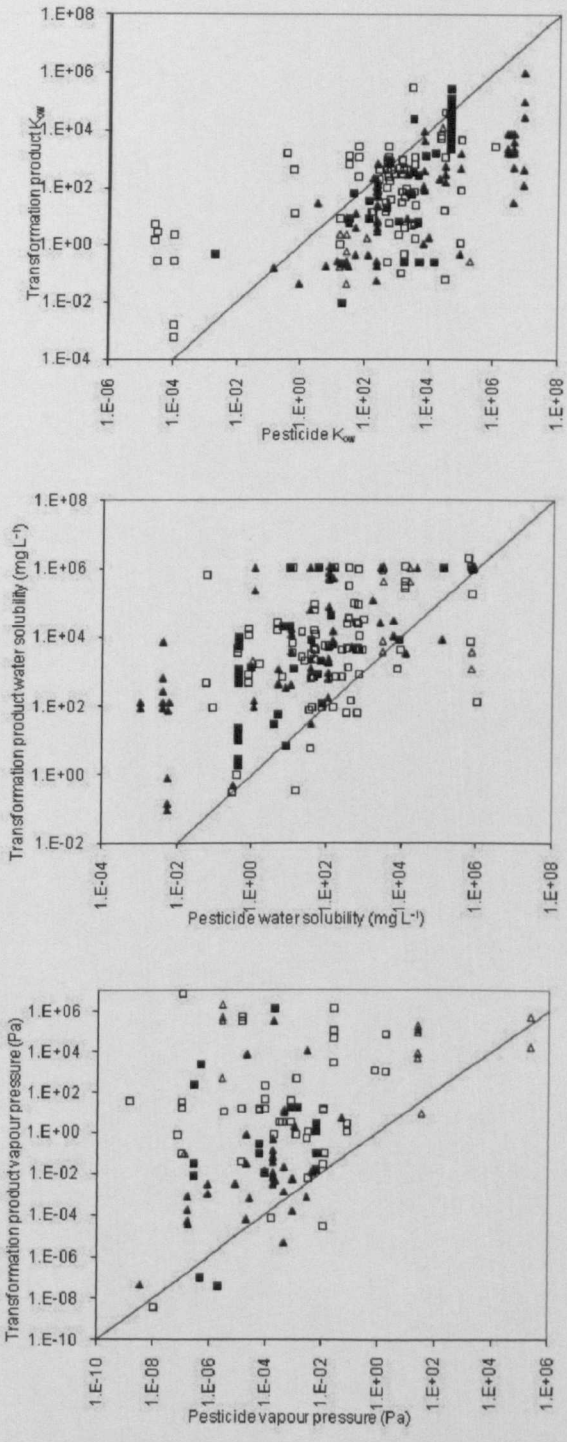

Figure 10. A comparison of physicochemical properties of pesticides and their transformation products (fungicides - ■; herbicides - □; insecticides - ▲; mixed mode of action - Δ) (line - x=y)

Herbicide and fungicide physico-chemical properties are very important for their uptake and translocation to the required site of action. Water solubility has been correlated to permeation through membranes (Ersoz et al. 1996), whilst water solubility, lipophilicity and dissociation are important for uptake by roots and xylem transport (Sicbaldi et al. 1997; Chamberlain et al. 1998). Approximately half (49.5%) of the transformation products were more than one order of magnitude more hydrophilic than their parent pesticides (Table 10). Only 6% of the transformation products formed from insecticides exhibited an increase in hydrophobicity, whereas 21% and 31% of transformation products of fungicides and herbicides respectively, exhibit the same increase. Transformation products of highly hydrophilic herbicides, e.g. $K_{ow} < 1$, were all more hydrophobic than their parents. Moreover only 5.2% and 7.7% of insecticidal and fungicidal transformation products respectively, were less water soluble than their parent pesticides, but none were less water soluble by more than an order of magnitude.

Table 10. Percentage of transformation product physico-chemical properties, one, two and three orders of magnitude greater than or less than their respective pesticide properties

Orders of magnitude	Water solubility	Hydrophobicity	Vapour pressure	Henry's law constant
Less				
3	0.6	14.3	0	10.7
2	1.7	26	1.8	14.3
1	4	49.5	3.5	21.4
More				
1	69.9	8.2	80.5	39.3
2	41.5	5.1	71.7	35.7
3	28.4	3.6	54	32.1
No. of comparisons	176	196	113	28

Available transformation product pKa values allowed 112 comparisons of dissociation with parent pesticides to be undertaken. Within this comparative data, 64% of the parent pesticides do not dissociate at all, whilst at pH 7 58% of the transformation products would be more than 50% dissociated. Comparisons between transformation products and pesticides that both dissociate (40/112), indicated that 90% of the pesticides and 62.5% of the transformation products would be more than 50% dissociated at neutral pH. Whilst, when pesticides that

do not dissociate and their transformation products are compared (72/112), 56.9% of the transformation products would be more than 50% dissociated at neutral pH. Therefore the dissociation of the parental pesticide has limited influence on the dissociation of subsequent transformation product(s).

3.3.3 Estimation of Transformation Product and Pesticide Properties

The determination of predictive ability for all techniques investigated generated extensive figures and tables which are provided in Appendix B. A summary of the best performing technique for each property for pesticide and transformation products is provided in Table 11.

Table 11. Summary of best performing approach for six properties (mean rank score)

Property	All compounds		Common compounds	
Transformation products				
K_{oc}	Kanazawa (1989)	(0.24)	Kanazawa (1989)	(0.25)
K_{ow}	KOWWIN	(0.41)	CLogP[a]	(0.4)
pKa	SPARC	(0.39)	SPARC	(0.32)
Water solubility	WSKOWWIN	(0.59)	WSKOWWIN	(0.68)
Vapour pressure	Mpbpwin	(0.59)	ASTER	(0.69)
Henry's law constant	Henrywin-bond	(0.71)	Henrywin-bond	(0.64)
Pesticides				
K_{oc}	Briggs et al. (1981)	(0.45)	Briggs et al. (1981)	(0.43)
K_{ow}	ALogPS	(0.46)	ALogPS	(0.52)
pKa	ASTER	(0.84)	SPARC	(0.57)
Water solubility	LogS	(0.52)	LogS	(0.57)
Vapour pressure	Mpbpwin	(0.59)	Mpbpwin	(0.68)
Henry's law constant	Henrywin-bond	(0.58)	Henrywin-bond	(0.57)

[a] – A combined approach was developed

3.3.3.1 Hydrophobicity

KOWWIN, CLogP, LogP, ALogPS and XLogP all had a tendency to under predict K_{ow}, whilst miLogP had a tendency to over predict (Figure 11; Table B1 in Appendix B), only the under prediction of XLogP was identified as being significant (95% confidence limits). KOWWIN, CLogP, LogP and ALogPS all had a mean rank score within 0.09 rank units of each other for predictions of all and common transformation products, indicating that their ability to provide

estimates for the transformation product dataset was similar. Moreover these four techniques also predict ≥95% of compounds to within one order of magnitude of experimentally determined values (Figure 11), XLogP and miLogP performed less well. When the techniques were evaluated for 'all' transformation products, KOWWIN was the best performing technique (mean rank score 0.41), whilst CLogP was the best performing technique for 'common' transformation products (mean rank score 0.4) (Table 9).

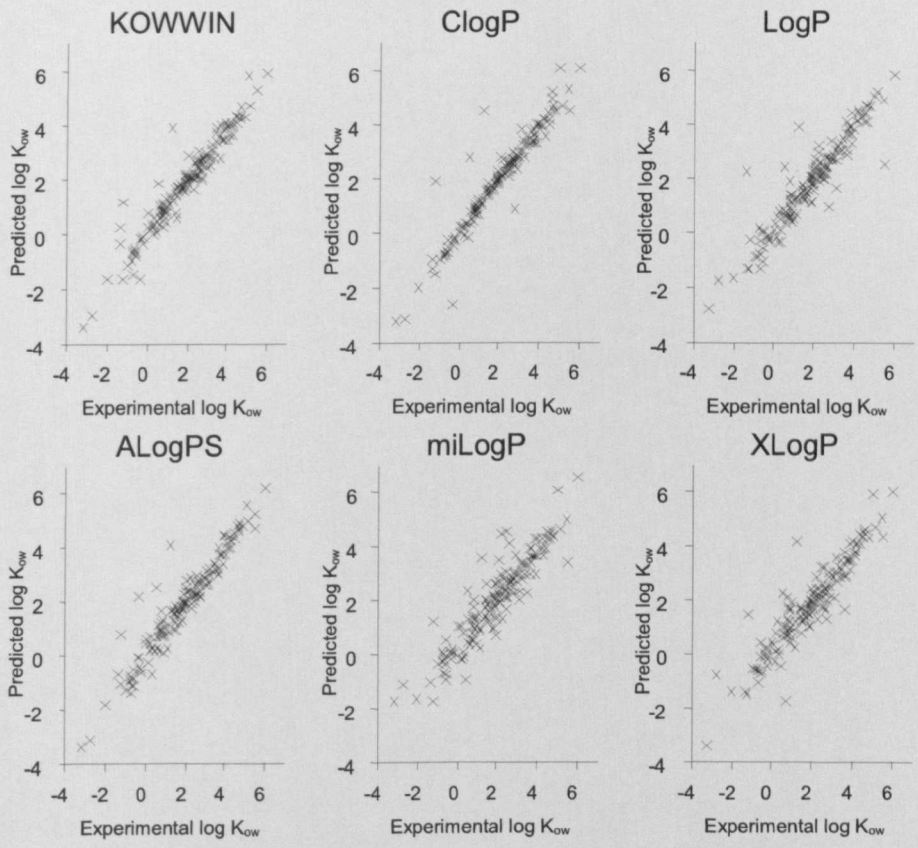

Figure 11. The predictive ability of six techniques for providing K_{ow} for transformation products (all compounds)

Independent evaluations have suggested that for pharmaceuticals CLogP outperforms KOWWIN (Mannhold and Petrauskas 2003; Machatha and Yalkowsky 2005), however these compounds are generally more complex than

transformation products, for simple organic datasets, similar to the complexity of transformation products considered here, performance was equivalent (Sakata et al. 1992) as demonstrated during this evaluation. Four transformation products were consistently under or over predicted by four or more approaches, suggesting that either the approaches can't accurately provide estimates for these compounds or experimentally collated data were inaccurate; bifenox anthranilic acid (bifenox), fluroxypyr (fluroxypyr-meptyl), 6-chloro-3-phenyl-pyridazin-4-ol (pyridate) and 2-(3,5-dichlorophenyl)-4,4-dimethyl-5-methyleneoxazoline (propyzamide).

It has been proposed that the prediction K_{ow} for agricultural chemicals can be significantly improved by combing the estimates from a number of different approaches (Clarke et al. 2004). Therefore all possible combinations of the four best performing techniques (KOWWIN, CLogP, LogP and ALogPS), from the individual method to a mean value from all four methods, were evaluated for the 156 'common' transformation products and evaluated statistically. This analysis indicated that predictions for the dataset could be improved using a mean value from estimates provided by KOWWIN, CLogP and ALogPS. This combined prediction enabled >98% of transformation products to be estimated to within one order of magnitude of experimentally determined values with a Pearson correlation coefficient of 0.971 (Figure 12; Table B3 in Appendix B). If the four transformation products that were consistently under or over predicted were removed then all estimates were within one log unit of experimental values (data not shown).

At the time of the evaluation these three approaches were freely available for use as a web-based front end or as a software download and can all be considered sub-structural approaches, KOWWIN and CLogP cleave query molecules into groups/fragments with K_{ow} estimated using atom and fragment contributions, whilst ALogPS uses atom and bond-type E-state indices as well as hydrogen atom numbers developed within a neural network to produce estimates. It has been suggested that sub-structural approaches continuously outperform those

that consider whole molecule (Mannhold and Petrauskas 2003; Sakuratani et al. 2007) since they do not have such a confined structural domain as whole-molecule approaches and are therefore applicable as long as the fragments/groups within the query molecules are covered and unlike whole molecule approaches are not susceptible to unknown effects (Mannhold and Petrauskas 2003). The combination of methods may perform better than any individual technique for a diverse range of compounds because this will 'smooth out' any problems an individual technique may have with certain compounds, group of compounds or compound fragments.

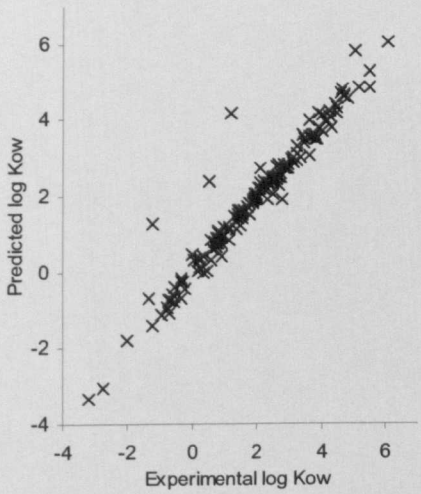

Figure 12. Estimation of transformation product hydrophobicity using a mean value from KOWWIN, CLogP and ALogPS

When pesticides were considered, none of the approaches performed as accurately as they had for transformation products (Figure B2 in Appendix B) ALogPS was the best performing technique (Table 9), however ~16% (n=71) of pesticides had their K_{ow} value predicted more than one log unit away from experimentally determined values. There were a number of pesticidal chemical classes where three or more pesticide predictions were more than one log unit away from experimentally derived values; arylphenoxypropionic acids (n=3), cyclohexanedione oximes (n=3), morpholines (n=3), aryloxyalkanoic acids

(n=4), organophosphorus insecticides (n=7), synthetic pyrethroids (n=8) and sulfonylurea herbicides (n=8).

3.3.3.2 Soil sorption

Eleven separate techniques were evaluated for providing soil sorption data, two software based approaches, seven linear relationships that use K_{ow} as the input parameter and two linear relationships that use water solubility as the input parameter (Table 8). The experimentally determined soil sorption data collected for pesticides and their transformation products generally comprised a range of values since the determination of this property can vary with soil properties, i.e. pH, clay content, organic carbon content and soil texture (OECD 2000). Minimum K_{oc} values were therefore selected as the parameter to evaluate predictive techniques against, since this was a consistent data parameter within the dataset available for the majority of compounds and represents 'worst-case' in terms of the mobility through the environment. Therefore it was anticipated that the techniques would over-estimate the minimum K_{oc} values if they had been developed using mean K_{oc} data.

As expected the majority of the evaluated approaches over-estimated minimum K_{oc} values for transformation products and pesticides (Table B10 in Appendix B). However the two linear relationship approaches that use water solubility as the input, Briggs (WS) (1981) and Kenaga and Goring (WS) (1980) consistently under-estimated minimum K_{oc} values. When common transformation products were considered, three of the evaluated approaches, Sabljić et al. (1995), Kanazawa (1989) and Briggs (1981) were proficient at providing minimum K_{oc} data. All these approaches used hydrophobicity as the input parameter, had mean rank scores within 0.5 units of each other, did not have a significant tendency to under or over predict minimum K_{oc} data and >96% of estimates where within one log unit (Table B10 in Appendix B).

Estimation approaches such as these, based on hydrophobicity, model sorption to organic carbon but do not consider other processes such as sorption to clay

minerals or the effects of pH (Doucette 2003). Since sorption behaviour is normalised for the organic carbon content, i.e. K_{oc}, then K_{ow} based techniques will provide accurate estimates when sorption to organic matter is the dominate process, where other sorptive interactions are important, i.e. providing larger values of K_{oc}, then estimates will be less accurate since not all the sorptive behaviour will be modelled. The sorption of neutral hydrophobic organic compounds could be well modelled by just considering the sorption to organic matter (Lambert et al. 1965; Chiou et al. 1979), whilst the influence of other process would need to be considered to accurately model the sorptive behaviour of ionic compounds (Kah and Brown 2007).

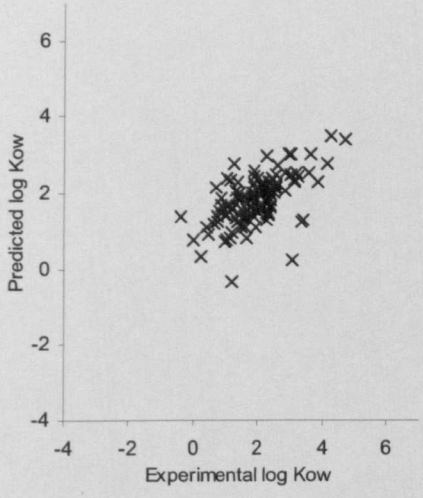

Figure 13. Estimation of transformation product minimum K_{oc} using the relationship of Kanazawa (1989)

An evaluation of whether a combination of the three best approaches for providing minimum K_{oc} data for transformation products would be more accurate than any individual approach was undertaken. This was carried out in the same manner as for the prediction of hydrophobicity, however during this evaluation the two transformation products estimated to be greater than one log unit away from experimental values, 2,4-D (2,4-DB) and dicofol (DDT) by all approaches, were removed from the analysis. Sorption estimates could not be improved by combing methods and the relationship of Kanazawa (1989) was still

the best performing relationship (Figure 13; Table B12 in Appendix B). Moreover, an attempt to increase the potential accuracy of this technique by highlighting potential outliers by the extent of their dissociation was undertaken. This analysis proved unsuccessful (results not provided).

Dearden (2004) undertook an assessment of methods for providing Koc estimates using an experimental dataset of 100. PCKOCWIN was selected as the best approach as it provided the most accurate predictions and is freely available to download from the internet. However during the current study the relationships of Sabljić et al. (1995) and Kanazawa (1989) were the most consistent performing approaches, not PCKOCWIN. It is possible that since Sabljić et al (1995) and Kanazawa (1989) were developed using agricultural chemicals then they are more relevant to pesticide transformation products than other general chemicals. The training set for Sabljić et al. (1995) is extensive, 216 compounds with log K_{ow} between 1-7, however the relationship of Kanazawa (1989) is based on data from just 15 pesticides (nine insecticides and six herbicides). Therefore it could be argued that the relationship of Sabljić et al. (1995) maybe the more appropriate to use to provide transformation products data because it has a larger prediction space. However during this evaluation it was the relationship of Kanazawa (1989) that out performed all other tested methodologies. When using such an approach to provide K_{oc} data for risk assessment or screening it may be advisable to incorporate a safety factor into the estimation. The relationships of Sabljić et al. (1995) and Kanazawa (1989) predict > 95% of minimum K_{oc} values to within one log unit, therefore a safety factor of 0.1 maybe appropriate. This would provide a conservative estimate of mobility for a transformation product where the user can be confident that the estimated value is lower than the actual value if it were determined experimentally.

When the pesticide dataset were considered none of the approaches were found to be as accurate as for the transformation products. The three most accurate approaches were Sabljić et al. (1995), Kanazawa (1989) and Briggs (WS) (1981).

No individual approach could predict greater than 82% of minimum K_{oc} values to within one log unit of experimentally derived data.

3.3.3.3 Additional properties

When estimating water solubility for transformation products, WSKOWWIN was the best performing technique (mean rank score 0.68) (Figure B3 & Table B4 in Appendix B), whilst LogS was the best performing technique for pesticides (mean rank score 0.57) (Figure B4 & Table B5 in Appendix B). However overall, the techniques performed relatively poorly, with no technique able to predict more than 80% of either dataset to within an order of magnitude of experimentally determined values and mean absolute deviation greater than 0.7 log units for all approaches/datasets. Throughout the evaluation ASTER was ranked behind the other approaches, achieving the highest mean score in all assessments.

When the estimation of vapour pressure was evaluated ASTER was the most accurate technique for providing data for transformation products (Figure B5 & Table B6 in Appendix B), whilst Mpbpwin was identified as the most accurate technique for providing data for pesticides (Figure B6 & Table B7 in Appendix B). Three transformation products, namely nitric acid, nitrogen dioxide and nitrogen tetraoxide from chloropicrin, drastically altered the overall ability of Mpbpwin. Mpbpwin estimated that these compounds, comprised solely of nitrogen and oxygen, were non-volatile which incorrectly estimated vapour pressure by at least 17 orders of magnitude. When removed from the evaluation the overall performance of Mpbpwin improved (data not shown), without these outliers Mpbpwin performed better than ASTER for estimating transformation product vapour pressure.

The evaluation of approaches for predicting henry's law constant values was hampered by the lack of experimental data for pesticides and transformation products. This evaluation had by far the smallest available dataset of any of the prediction approach evaluations (Table 9). The bond-contribution method of

Henrywin had the lowest rank score for all compound datasets evaluated (Table B6 & B7 in Appendix B). This approach provided predictions for 100% and 98% for transformation products and pesticides respectively whilst the group-contribution method could only provide predictions for 68% and 23% respectively. When the common datasets were evaluated the bond contribution method of Henrywin was determined as the best performing approach for transformation products and pesticides.

When estimating dissociation, SPARC can provide the user with more than one pKa value for each compound examined, since pKa values are provided for each reaction centre in the molecule (Karickhoff et al. 1991). Where compounds had more than one estimate they where removed from the subsequent statistical analysis since it would be difficult to determine which of the predicted values should be considered when using the approach for an unknown compound. A prediction of non-ionisation was assumed when; a negative estimate of pKa was provided, the approach did not identify a reaction centre in the molecule or the output was 'non-applicable'.

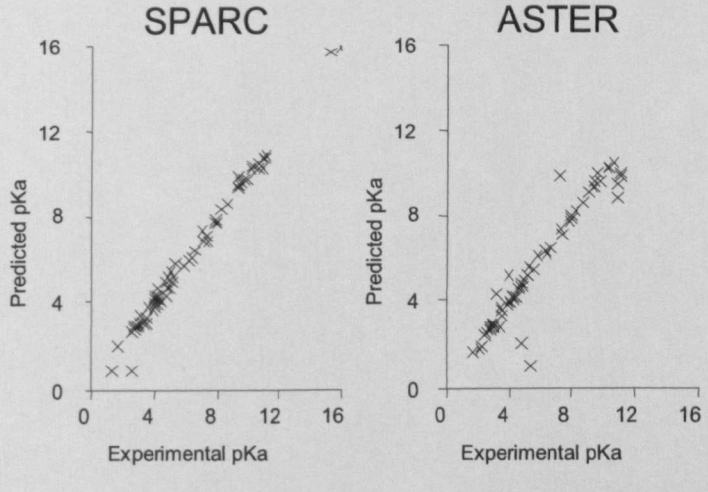

Figure 14. A correlation between experimental pKa values those estimated by SPARC and ASTER for transformation products (all compounds)

When dissociation was estimated for transformation products, SPARC and ASTER predicted that 6.7% and 17.8% respectively, would not dissociate, when experimental data proved otherwise. SPARC provided more than one pKa value for 18 transformation products (20%) and was the best performing technique (Figure 14). When common transformation products were evaluated, all SPARC predictions were within one pH unit of experimentally determined values and the Pearson correlation coefficient was 0.996. This evaluation demonstrates that SPARC is a very accurate tool for providing dissociation data for pesticide transformation products in accordance with previous evaluations (Hilal and Karickhoff 1995).

Experimental data were available on 279 pesticides that do not dissociate and ASTER correctly predicted that 94.3% (n = 263) of these compounds would not dissociate whilst SPARC provided pKa estimates for 17.6% (n = 49). When pesticides with experimentally derived pKa values were considered, SPARC and ASTER predicted that 52.8% and 31.9% would not dissociate. In comparison to transformation product estimates both approaches performed poorly in providing accurate pKa values for pesticides (Figure B10 in Appendix B).

Degradation of organic chemicals in soils, like sorption, is heavily influenced by the soil and experimental conditions. The predictive approaches assessed during this study provide degradation estimates quantitatively, qualitatively and as a probability. Therefore the ability of each approach was examined individually and not compared. Predictive approaches were evaluated against the 'worst-case' data, i.e. the maximum degradation data available for a compound. An evaluation for degradation of pesticides was not undertaken. BIOWIN contains three separate degradation models. During this evaluation two of those approaches were evaluated. The primary degradation survey model provides a qualitative prediction, e.g. days - weeks, whilst the biodegradation model (linear and non-linear) provides the user with a probability of biodegradation. Using information provided in the user manual this probability can be converted to a 'does not biodegrade' or 'biodegrades fast' categorisation.

The primary degradation survey model did not accurately provide any estimates for aerobic soil degradation. Transformation products categorised by the model as degrading within days-weeks had maximum experimental degradation rate constants spanning less than a day to greater than a thousand days (Figure 15). Similarly no correlation was observed between transformation product soil degradation data and the linear and non-linear biodegradation models (Figure B14 in Appendix B). Transformation products with experimental aerobic soil degradation rate constants that range from less than a day to greater than one thousand days were allocated to both the degrades fast and does not biodegrade categories.

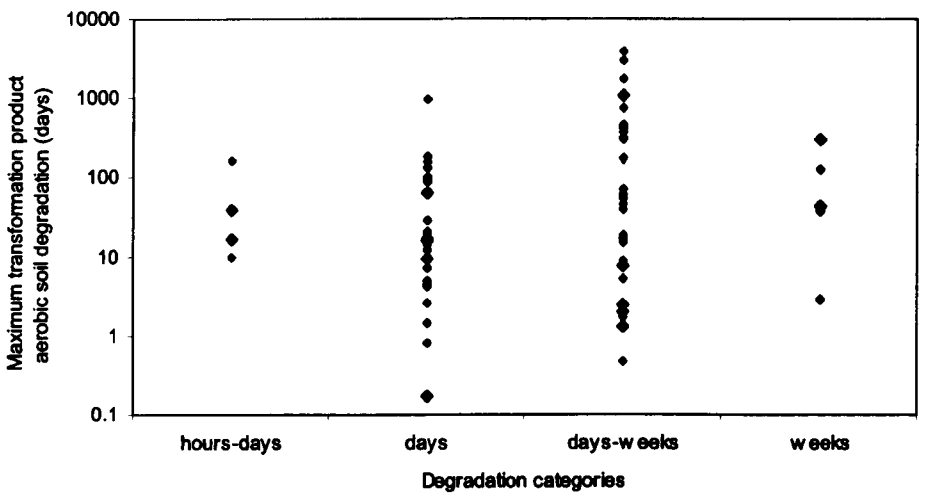

Figure 15. The predictive ability of the BIOWIN primary degradation survey model evaluated against experimental transformation product aerobic soil degradation rate constants

The second approach evaluated for estimating aerobic soil degradation rate constants for transformation products was the PBT Profiler which allocated all the transformation products to aerobic soil degradation rate constants of either 30, 75, 120 or 360 days and uses the ultimate degradation model of BIOWIN to estimate degradation.. A correlation between the median experimental

degradation rate constants and the predicted values (r^2 = 0.981) was observed, however this correlation fell down when the mean data values were examined (r^2 = < 0.1).

3.4 Conclusions

When physico-chemical properties of transformation products are compared to their parental pesticides, they indicate that these compounds will be more mobile in the environment since they are less hydrophobic, more water soluble and more volatile than their respective parent pesticides. Generally transformation products are more hydrophilic than their respective parent pesticides but there are exceptions, transformation products of hydrophilic herbicides were all more hydrophobic than their parental pesticides. The properties considered here are both important for quantifying the mobility of a compound through the environment as well as determining the fate during drinking water treatment processes. Therefore it is important that the fate of transformation products in the environment and fate during water treatment are considered when investigating the risk to ecosystems and humans of parent pesticides.

When approaches where evaluated for estimating water solubility, vapour pressure, henry's law constant and soil degradation performed poorly. Whilst estimates of hydrophobicity and dissociation were extremely accurate with the accuracy of pesticide transformation products hydrophobicity estimates increased by combining the predictions from three freely approaches, KOWWIN, ALogPS and CLogP. Moreover, SPARC is recommended as the technique for estimating dissociation since it performed extremely well for the diverse range of transformation products present in the evaluation dataset. The linear relationship of Kanazawa (1989) based on just sixteen pesticides out performed all other approaches evaluated for estimating a conservative minimum K_{oc} value for transformation products. When using this approach it may be useful to employ a safety factor of 0.1 to provide a conservative estimate. Therefore for certain important properties predictive approaches may offer a low

cost tool for rapidly providing data for transformation products in the absence of experimental data which could be used for risk assessment and/or prioritisation exercises. However for certain properties such as water solubility, vapour pressure and soil degradation rate constants the accuracy of the tested approaches was poor. This is unfortunate since these are properties that are often required when using higher-tier exposure models. There is therefore a requirement to further develop approaches to increase their ability to estimate these properties for transformation products.

The lack of an appropriate tool to provide accurate estimates of soil degradation rate constants was very disappointing as this can be the crucial property when determining the fate of a compound in the environment. Unlike other physico-chemical properties the result of soil degradation rate constant studies can be highly influenced by experimental conditions. Whilst certain parameters are easy to control through the use of appropriate laboratory equipment (e.g. temperature and humidity) and the selection of appropriate soils (e.g. soil pH, organic carbon content and clay content), the activity and diversity of microbial populations is difficult to quantify and standardise. However attempts have been made to provide standard soils for use during regulatory risk assessment studies (Kuhnt and Muntau 1994) and result variability is limited within experimental study protocols that stipulate the number and properties of soil used. However, during the development of predictive approaches, an average degradation rate constant per chemical from a number of soils is used in the training set. This ignores a whole level of important appropriate data on soil properties that could be utilised in the development of better techniques. There must be scope to develop more accurate approach(es) by using the extensive data available for pesticides and transformation products and combining this with targeted experimental studies.

3.4.1 Appendices

Extensive supporting information is available in Appendix B this includes all correlations between experimental and estimated data for all properties and approaches evaluated using common transformation product and pesticide datasets. Moreover all derived statistics and mean rank scores are also available.

4 Assessing the Ecotoxicity of Pesticide Transformation Products[1]

4.1 Introduction

When released to the environment, pesticides may be degraded either by micro-organisms or chemical processes (Roberts 1998; Roberts and Hutson 1999). Generally pesticide transformation products will have a lower toxicity to biota than the parent compound (Stratton 1981; Day and Maguire 1990; Day and Hodge 1996). However, in some instances a transformation product may be more toxic and consequently these substances may pose a greater risk to the environment than the parent compound (Stratton and Corke 1982; Osano et al. 2002a; Osano et al. 2002b). Differences in the environmental behaviour of many transformation products compared to the parent, e.g. where a transformation product may have increased mobility compared to the parent (Kolpin et al. 2001), could also mean that even when a transformation product is less toxic it may still have the potential to have an adverse impact on the environment. Consequently there is a need to consider transformation products during the environmental risk assessment process. In Europe, under EU Directive 91/414/EEC (European Commission 1994) and its subsequent amendments, data must be provided for all metabolites, degradation and reaction products which account for more than 10% of the amount of active substance added. Guidance on assessing the relevance of transformation products has been developed (European Commission 2002a; European Commission 2002b; European Commission 2003).

The effect of a compound on an organism will be dependent on the individual chemical and the interaction between that chemical and the species of interest (Bradbury 1994; Wroath and Boxall 1996). There are a number of possible explanations for a transformation product being more toxic than its parent

[1] Sinclair C.J. and Boxall A.B.A. (2003) Assessing the ecotoxicity of pesticide transformation products, Environmental Science and Technology, 37:4617-4625.

compound: 1) the active moiety of the parent compound is still present in the transformation product and hence the transformation product has the same toxic mechanism as the parent; 2) the transformation product is the active component of a pro-pesticide, where the applied substance is designed to be absorbed by an organism and once absorbed is metabolised to an active substance that elicits the desired effect (Drabek and Neumann 1985); 3) the bioconcentration factor for the transformation product is greater than the parent and hence more will reach the site of action. This is a key factor affecting the ecotoxicity of compounds which act via a similar mode of action (Lipnick 1990; Escher and Hermens 2002); and 4) the transformation pathway results in a product with a different and more potent mode of action than the parent compound. Differences in toxicity between pesticides and their transformation products could also be due to the variability inherent in toxicity testing.

If information on the modes of action of parent compounds and transformation products can be obtained and differences in accumulation can be determined, it may be possible to identify at a very early stage, which transformation products require testing. This study was therefore performed to determine whether the environmental effects of pesticide transformation products can be estimated based on data for the parent compound and information on structure in order to develop a pragmatic approach for their identification and risk assessment. The specific objectives of the study were to: 1) collect and collate available data on pesticide transformation products; 2) provide a qualitative means of identifying transformation products which maintain the specific toxic mechanism of their parental pesticides; 3) investigate the relative ecotoxicity to non-target organisms of pesticide transformation products compared to their associated parent compound; and 4) derive a framework for estimating the effects of transformation products on the environment.

4.2 Materials and Methods

4.2.1 Data collation

Initially, an extensive search was undertaken to identify the environmental degradation products of a wide range of pesticides. The majority of the degradation products and pathways were identified using the reviews of Roberts (1998) and Roberts and Hutson (1999) and disclosure documents produced for individual active substances by the UK Pesticides Safety Directorate (PSD 2003). Only those transformation products that are formed by biological, chemical and/or physical processes in soil, water, sediment or air were selected. Transformation products formed solely as a product of metabolism by plants and/or animals were not considered. If a compound was identified to occur as a result of pesticide degradation it was assessed, no matter what amount relative to the parent compound was formed during the transformation process.

Once structures of the transformation products had been identified data were collected on the physico-chemical properties (pKa, log K_{ow} and log K_{oc}), ecotoxicity and fate and behaviour of both pesticides and their transformation products. Data were collected from multiple sources including the open literature, databases such as the USEPA ECOTOX database (EPA 2003a), the IUCLID database (ECB 2000), the EFDB and PHYSPROP databases (SRC 2003a; SRC 2003b), PSD disclosure documents (PSD 2003) and the report by (Belfroid et al. 1996).

The ecotoxicity data obtained covered a wide range of test species and endpoints. Moreover, multiple values were often available from a number of sources for a particular endpoint. Only a limited amount of information was available on the chronic effects of the transformation products, effects on aquatic macrophytes and effects on terrestrial organisms. Therefore, for comparative reasons, only data derived from acute tests using fish, daphnids and algae and following OECD guidelines (OECD 1984a; OECD 1984b; OECD 1992) were selected for

further analysis. An algal endpoint (72-96h EC_{50} population), not detailed in the OECD guidelines was included to increase the number of algal data points.

As many of the data points were obtained from online databases that cite data from the published literature, it was necessary to assess the accuracy of the citations. As a large amount of information was obtained it was impractical to assess all data points by obtaining the original data source that was cited in the database. The original citation was only obtained in the following instances: 1) when a large number of data points were available on a particular substance from a number of sources and where the values for one or more of the data points exhibited a large difference compared to the majority of the data points; and 2) when three or fewer data points were reported for a particular substance. If appropriate, the data were revised in light of the results of the quality assessment. All assessed data were then entered into an Accord for Excel Version 5.0 spreadsheet (Accelrys Inc. 2001) which was used for subsequent analyses. Where multiple data points were available for a particular endpoint, the median value was calculated and used in the analyses.

4.2.2 Comparison of toxicity values of parent and transformation product

The ecotoxicity data for transformation products and their parent compound were compared to determine whether the transformation products had similar ecotoxicity or were more or less toxic. All of the transformation products were then examined, using the approaches described below, to determine which contained a toxicophore (a chemical moiety that is necessary for a specific toxic mechanism), which were more hydrophobic or less dissociated and which might have a more potent mode of action than the parent compound.

4.2.3 Identification of transformation products containing toxicophores

The specific toxic action of a pesticide is due to an interaction between a target site in the organism and the active moiety or toxicophore of the pesticide (Rand et al. 1995). Toxicophores for each of the major classes of pesticide were identified by looking for sub-structural similarities within a pesticidal class. The Pesticide Manual (Tomlin 1997) was used as a basis for this work. The structure of each transformation product for which ecotoxicity data were available was then examined to determine whether or not it contained a pesticide toxicophore.

4.2.4 Identification of transformation products with increased accumulation

Accumulation has been shown to relate to hydrophobicity and dissociation of a compound (Könemann 1981; Esser and Moser 1982; Hermens et al. 1984). Therefore to determine whether increases in ecotoxicity observed for many of the transformation products could be explained by increases in accumulation, the octanol-water partition coefficients (which give a measure of hydrophobicity) and acid dissociation constants (which provide an indication of the degree of dissociation of a substance at neutral pH) for parent compounds and transformation products were compared. Generally experimentally-determined values were used. However, in instances where experimental data were not available for log K_{ow} or pKa, the values were predicted, based on chemical structure, using KOWWIN v 1.6 (Meylan and Howard 1995; Meylan and Howard 1999) for K_{ow} and SPARC (Karickhoff et al. 1991) for pKa. Transformation products that had a greater K_{ow} value than their parent or which were less dissociated than the parent were considered likely to bioaccumulate to a greater extent than the parent.

4.2.5 Identification of toxic modes of action for transformation products

The structures of each of the transformation products were examined to determine whether or not they might be expected to have a reactive mode of action (Bradbury 1994). Three 'rule-based' approaches were used (Lipnick 1991; Verhaar et al. 1992; Russom et al. 1997). Each approach identified structural fragments associated with a range of modes of action, if one of these fragments was contained in the molecule of a transformation product and not in the parent compound then it was assumed that the product might have the mode of action associated with the fragment and that it might be more toxic than the parent.

4.3 Results and Discussion

Using the search strategy, information was obtained on the transformation pathways of 60 active compounds and based on these pathways the structures of 485 transformation products were identified. The active compounds examined covered a range of chemical classes and included 27 herbicides, 20 insecticides, 12 fungicides and one compound used as a herbicide, fungicide and insecticide. All the major classes of pesticide were represented by at least one active compound.

Table 12. Summary of the data available for parent compounds and their transformation products

Physico-chemical property/ Taxonomic group	Number of parents	Number of transformation products
log K_{ow}	36	71
pKa	35	64
log K_{oc}[a]	12	33
fish	30	60
daphnids	27	57
algae	11	16

[a] - These data were analysed independently with a different dataset

The final database (Table C1 in Appendix C) only comprised property and ecotoxicity values for 89 transformation products arising from 37 parent compounds. Twenty-three parent compounds with identified transformation pathways had either no corresponding data or only unsuitable data for their respective transformation products. Log K_{ow} values were available for 71 transformation products, pKa values were available for 64 transformation products and K_{oc} values were available for 33 transformation products (Table 12). In terms of the ecotoxicity data, fish 96h LC_{50} values were available for 60 transformation products, daphnid 48h EC_{50} values were available for 57 transformation products, whilst only 16 transformation products had acute algae ecotoxicity data (Table 12).

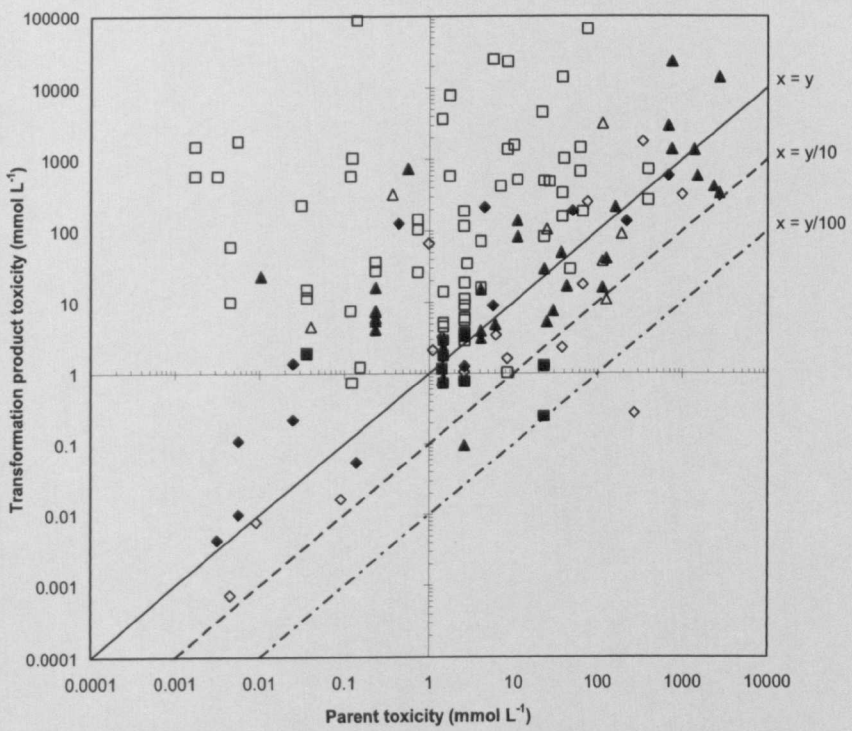

Figure 16. Generalisation between the ecotoxicity (to fish, daphnids and algae) of parent compounds and their transformation products that a) contain a toxicophore (black diamonds), b) are pro-pesticides (white diamonds), c) are more hydrophobic than the parent (black triangles), d) are less dissociated than the parent (white triangles), e) might be expected to have a more potent mode of action (black squares), or f) exhibit none of these characteristics (white squares)

A comparison of parent and transformation product ecotoxicity data (Figure 16) demonstrated that the majority (70%) of transformation products have either a similar toxicity to the parent compound or are less toxic. However, a significant proportion (30%; Table 13) are more toxic than their parent compound and 4.2% of transformation products are more than an order of magnitude more toxic. In terms of ecotoxicity values, in only 20 instances did a transformation product have an acute toxicity value of less than 1mg L^{-1}, one of the threshold values used in classifying chemicals in the EU, typically separating the classes 'very toxic' from 'toxic' (ECB 2003).

Table 13. Possible explanations for increases in toxicity observed for the transformation products for a) fish (F), b) daphnids (D) and c) algae (A)

Parent compound	Pesticidal class[a]	Transformation product	Toxicophore present	Pro-pesticide	Increase in hydrophobicity	Decrease in dissociation	Change in mode of action	Unknown
2,4-D	aryloxyalkanoic acid	2,4-dichlorophenol			F, D			
		4-chlorophenol				F, D, A		
		4-chlorocatechol				F		
acephate	organophosphorus	methamidophos		F, D				
aldicarb	oxime carbamates	aldicarb sulfone	D					
atrazine	1,3,5-triazine	deisopropyldeethyl atrazine	D					
azocyclotin	organotin	cyhexatin		F, D			F	
butylate	thiocarbamate	diisobutylamine						D
carbaryl	carbamates	1,4-dihydroxybenzene					F	
		5-hydroxy-,1,4-naphthoquinone						
dazomet	methyl isothiocyanate precursor	hydrogen sulphide						F
		methyl isothiocyanate		F, D, A				
diuron	urea	3,4-dichloroaniline			D			
fluometuron	urea	3-trifluoromethyl benzenamine			D			
fluridone	-	m-(trifluoromethyl) benzaldehyde			F			
gamma HCH	organochlorine	1,2,3,5-tetrachlorobenzene			D			
		alpha-HCH			D			
glyphosate	-	formaldehyde			D			

Table 13. Possible explanations for increases in toxicity observed for the transformation products for a) fish (F), b) daphnids (D) and c) algae (A)

Parent compound	Pesticidal class[a]	Transformation product	Toxicophore present	Pro-pesticide	Increase in hydrophobicity	Decrease in dissociation	Change in mode of action	Unknown
Continued...								
napropamide	alkanamide	1-naphthol						F
parathion	organophosphorus	paraoxon		F, D				
quinmerac	quinoliecarboxylic acid	BH-518-2	A					
quintozene	aromatic hydrocarbon derivative	2,3,4,6-tetrachlorophenol					D	
		2,3,5,6-tetrachlorophenol					F	
		3,4,5-trichlorophenol						D
		pentachlorophenol			F			
		pentachloroanisole			D			
rimsulfuron	sulfonylurea	IN-70942			D			
tecnazene	-	2,3,4,5-tetrachloroaniline					F	
		2,3,5,6-tetrachlorothioanisole			F			
thiodicarb	oxime carbamates	methomyl	D					
triclopyr	arloxyalkanoic acid	3,5,6-trichloro-2-pyridinol			F			
triflusulfuron-methyl	sulfonylurea	IN-D8526-2			F			
zineb	alkylenebis (dithiocarbamates)	ethylenethiourea		A				

[a] - from Tomlin (1997)

Fifty-four toxicophores associated with a wide range of pesticide classes were identified (Figure 17). It was not possible to identify a toxicophore for all the active compounds considered in the study. Some classes contained too few members within their pesticidal class for reasonable toxicophore identification, whilst some compounds had an undefined mode of action and/or were not a member of a defined pesticidal class.

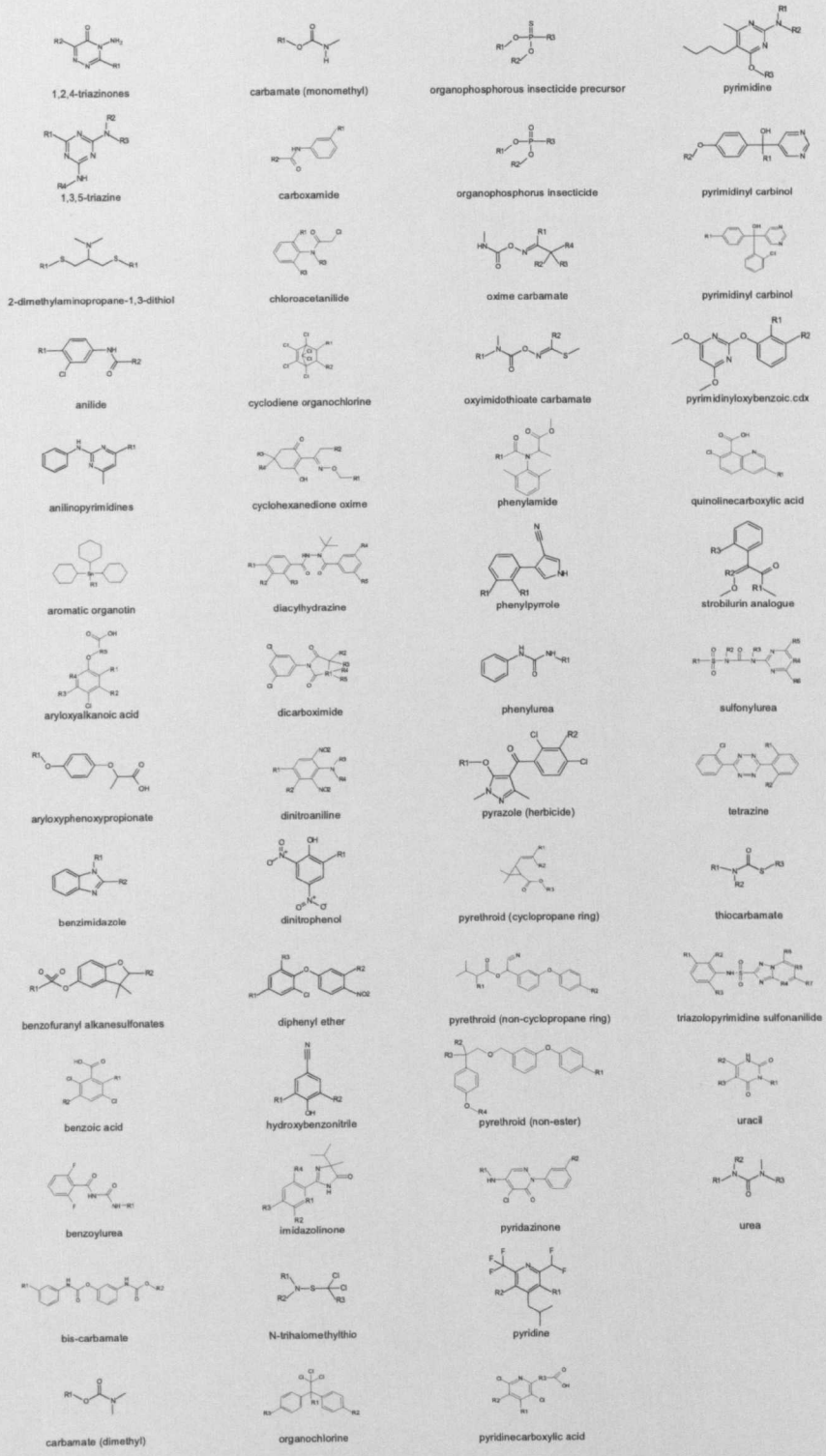

Figure 17. Toxicophores identified for major pesticide classes

When those substances identified as having increased toxicity in relation to their parent compound were evaluated it was found that over 90% of the observed increases in toxicity could be explained by the presence of a toxicophore, differences in accumulation or differences in mode of action (Table 13; Figure 16). Four substances still contained the parent toxicophore, five substances were the active substances resulting from a pro-pesticide, 13 substances were more hydrophobic than their parent compound and two substances would be expected to be less dissociated than their parent compound. Five substances would have a reactive mode of action or act via respiratory uncoupling; these were 5-hydroxy-1,4-naphthoquinone, 1,4-dihydroxybenzene, tetrachloroaniline, 2,3,4,6-tetrachlorophenol and 2,3,5,6-tetrachlorophenol. 5-hydroxy-1,4-naphthoquinone and 1,4,-dihydroxybenzene are known to be highly reactive (Verhaar et al. 1992; Russom et al. 1997). The high toxicity of quinones has been attributed to enzymatically based redox cycling resulting in superoxide formation and the regeneration of the quinine (Mason 1990). It has been suggested that the 1,4-dihydroxybenzene can be oxidised to a quinone and thus exhibit the same futile metabolism (Cronin Pers. Comm. 2003). Tetrachloroaniline and tetrachlorophenol are uncouplers of oxidative phosphorylation (Russom et al. 1997). For transformation products that did not have a specific mode of action (i.e. did not contain a toxicophore or are active component of a pro-pesticide), the difference between the toxicity of the parent and the toxicity of the transformation product appeared to depend on the potency of the parent. In situations where a parent compound was highly potent the difference between toxicity values for the parent and transformation product was large whereas in situations where the parent compound was less potent the difference between the parent and transformation product was small. One possible explanation for this is that most transformation products, after having lost the active moiety, exhibit baseline toxicity, which is considerable lower than the specific toxic effects of the pesticides.

Whilst, information on accumulation and mode of action explained the increases in toxicity for a significant proportion of the transformation products, a large

proportion (30%) of products that were less toxic than the parent compound also had one or more of the characteristics. Many of these observations could however be explained by the following:

1) The presence of a toxicophore in a transformation product does not necessarily mean that the substance will be more potent than the parent compound. For example, the product may still have pesticide activity but be accumulated to a lesser extent than the parent.

2) The presence of a toxicophore in a molecule does not always mean that the molecule will have pesticidal activity. For example, interactions with other functional groups in the molecule may mean the toxicophore cannot interact with the site of action.

3) The mode of action of the toxicophore may not be relevant for certain test species. For example, a substance containing a herbicidal toxicophore would not be expected to exhibit an increase in toxicity to fish and daphnids. Data for the pro-pesticides support this. For insecticidal pro-pesticides increases in toxicity of the transformation products were observed in fish and daphnids whereas for herbicidal and fungicidal pro-pesticides, the transformation products were less toxic than their parents to fish and daphnids.

4) A transformation product that is more hydrophobic than its parent compound and does not have pesticidal activity is unlikely to be more toxic than its parent to sensitive species that have a receptor site relevant to the parent mode of action. Examination of the dataset supports this and indicates that transformation products which are more hydrophobic than and do not contain the parent toxicophore of an insecticide parent compound are generally less toxic than the parent to fish and daphnids. Similarly, transformation products not containing a toxicophore and which are more hydrophobic than a herbicide parent compounds are generally less toxic than the parent to algae.

5) A transformation product that is less dissociated than its parent may also be much less hydrophobic, the effect on accumulation of the decrease in dissociation may therefore be offset by the reduction in hydrophobicity. This may explain why succinic acid is less toxic than 2,4-D even though it is less dissociated, succinic acid has a log K_{ow} of -0.6 compared to a log K_{ow} of 2.81 for 2,4-D.

Therefore, when assessing the potential impacts of a particular transformation product, ideally as much information as possible should be used on the mechanism(s) of action of the parent, the sensitivity of the different taxa to the parent compound and the properties of both the parent compound and the transformation product.

The availability of data has meant that it has been only possible to investigate the relationships between acute aquatic toxicity endpoints (for fish, daphnids and algae) for parent compounds and their transformation products. Recent studies using chronic data for aquatic species and data for terrestrial organisms (Maroni et al. 2002) indicate that when these endpoints are considered, parents are generally of equal toxicity to or are more toxic than their transformation products. However, as in the current study, there were instances where a transformation product was more toxic than the parent compound. Unfortunately, the studies are based on confidential data so it is not possible to determine whether the factors that explain the increases in acute aquatic ecotoxicity values used in the present study also explain the increases in chronic or terrestrial ecotoxicity.

4.4 A pragmatic method for estimating ecotoxicity

The findings described above indicate that it is possible to begin to prioritise transformation products based on information on mode of action and accumulation. On the basis of the results obtained it is possible to begin to develop a framework that might be used to assess the potential effects of

transformation products on aquatic organisms. A three-step process is proposed (Figure 18) which uses information on parent toxicity, transformation product structure and properties along with assessment factors. The assessment factors were derived from the ecotoxicity data using a cautious systematic approach which ensured that all data-points were covered. The assessment factors were generated by creating a series of 'bins'. These 'bins' were identified using the ecotoxicity comparison data and, for ease of use, ranges of parent toxicity values and assessment factors were selected to be factors of 10.

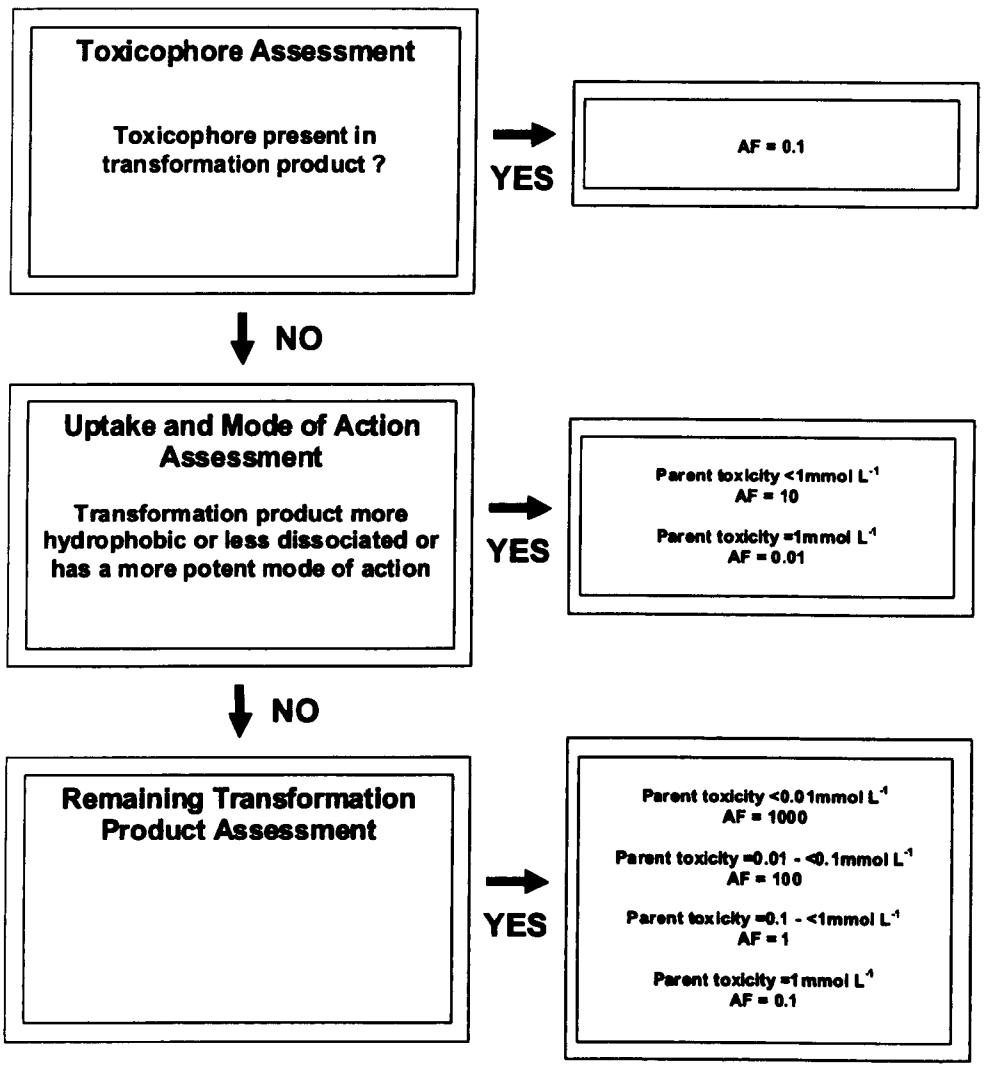

Figure 18. Flow chart summarising proposed transformation product assessment approach

4.4.1 Step 1 – Toxicophore assessment

The structure of the transformation product should be examined to determine whether it contains the parent toxicophore. If the parent toxicophore is present, then the effect of the transformation product can be estimated from ecotoxicity data for the parent compound using Equation 1 and an assessment factor (AF) of 0.1 (i.e. transformation products which maintain the toxicophore of the parent can be ten times more toxic than the pesticide). The AF is derived from the relationship between parent toxicity values and the difference between parent

and transformation product toxicity for substances containing the toxicophore (Table 14; Figure 19). In Figure 19 increThe toxicity endpoint for the parent ($LC/EC/IC_{50}$) used in Equation 1 should be that for the most susceptible species (fish, daphnids and algae) to the parent pesticide.

Equation 1. $$LC/EC/IC_{50\,transformationproduct} = LC/EC/IC_{50\,parent} * AF$$

Table 14. Assessment factors for determining $LC/EC/IC_{50}$ values of transformation products during the assessment scheme

$LC/EC/IC_{50}$ for parent compound (mmol L^{-1})	Assessment factor (AF)
Step 1	
Any value	0.1
Step 2	
<1	10
≥1	0.01
Step 3	
<0.01	1000
≥0.01 - <0.1	100
≥0.1 - <1	1
≥1	0.1

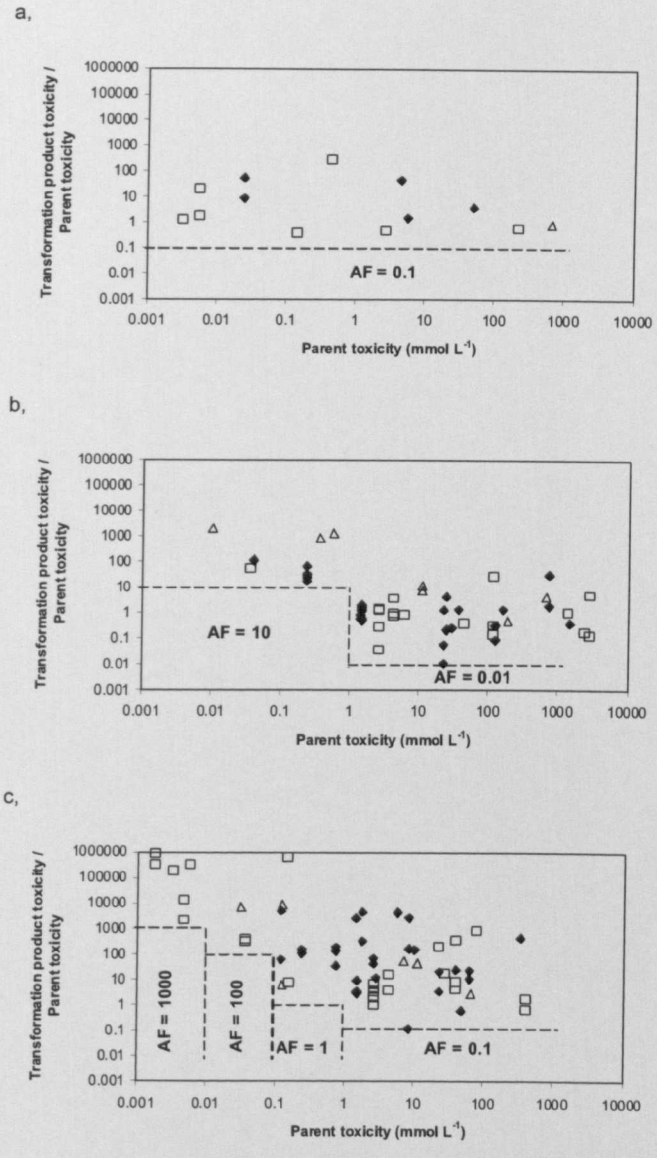

Figure 19. Relationship between parent ecotoxicity values (mmol L^{-1}) and the difference between parent and transformation product toxicity values for; fish (black diamonds), daphnids (white squares) and algae (white triangles) for a) transformation products containing a pesticide toxicophore; b) transformation products that are more hydrophobic, less dissociated or have a more potent mode of action than the parent; and c) the remaining transformation products. The the higher the value of the y-axis the less potent the transformation product toxicity is compared to the parent pesticide

4.4.2 Step 2 – Assessment of accumulation and mode of action

Those substances that do not contain the parental toxicophore are then assessed to determine whether: 1) the product is more hydrophobic than the parent compound; 2) the product is less dissociated than the parent compound; or 3) the product has a different but more potent mode of action than the parent compound. To determine the hydrophobicity (Kow) of the parent compound and the transformation product it is recommended that SRC's KOWWIN software is used to estimate the octanol-water partition coefficient. Whilst it is recommended that SPARC is used to determine dissociation. The rule based systems of Lipnick (1991), Verhaar et al. (1992) and Russom et al. (1997) should be used to determine whether a transformation product has a reactive mode of action or whether it is a respiratory uncoupler. Such rule based systems were not necessarily developed for pesticides and their transformation products so may not be appropriate for all occasions.

For all compounds that are shown to be more hydrophobic, less dissociated or which have a more potent mode of action than the parent compound, the assessment factors listed in Table 14 should be used along with Equation 1. The assessment factors have been derived from the relationship between parent toxicity and the difference between parent and transformation product toxicity for transformation products that are more hydrophobic, less dissociated or which might be expected to have a more potent mode of action (Figure 19) – this overcomes the issue of species sensitivity. All compounds that are less hydrophobic than the parent, equally or more greatly dissociated and which do not have a reactive mode of action or are not respiratory uncouplers, should move on to Step 3 assessment.

4.4.3 Step 3 – Assessment of remaining products

The effects of all remaining transformation products should be determined based on the ecotoxicity data for the parent compound using assessment factors and

Equation 1. The assessment factors (Table 14) have been derived from the relationship between the toxicity of the parent compound and the difference between the toxicity of transformation product and parent for all compounds that do not contain a toxicophore, which would not be expected to accumulate to a greater extent than the parent and which would not be expected to have a more potent mode of action (Figure 19).

Such an approach is precautionary. As information on the hydrophobicity and dissociation of transformation products can be accurately predicted from chemical structure using quantitative structure-property relationships (QSPR's) (Sinclair and Boxall 2002b), the only information required to perform the assessments are the structures of the transformation products for the substance of interest and experimental ecotoxicity values for the parent compound. The methodology could therefore be used at an early stage in the risk assessment process to identify transformation products that might pose a risk to the environment. These compounds could then be taken forward for experimental testing. The application of an approach of this type will result in clear cost and time savings and will minimise the use of laboratory animals.

The scheme and the assessment factors proposed are based on a limited dataset and whilst the dataset does cover a range of pesticide classes and modes of action, evaluation and validation against additional data would be beneficial and could allow further refinement of the methodology. This would probably be a requirement if the approach is to be adopted by regulatory authorities. Other studies into the effects of transformation products (Maroni et al. 2002; European Crop Protection Association 2002) have had access to unpublished data produced by industry and these indicate that a large body of data has been generated that could be used for evaluation purposes. These datasets not only include information on acute toxicity to fish, daphnids and algae but also include data on aquatic plants, sediment dwellers, earthworms and chronic endpoints.

The assessment process focuses solely on the determination of the potential effects of a particular transformation product. In order to identify transformation products that might pose a risk to the environment, it will also be necessary to assess exposure. Work has been done assessing the overall persistence and environmental concentrations in different compartments for solvent, surfactant and herbicidal transformation products (Fenner 2001). The development of approaches to assess exposure was beyond the scope of this study. In order to perform such assessments, information will be required on the persistence and mobility of transformation products. Assessment of currently available QSPR's for determining the sorption of a transformation product in soil or sediment systems, indicate that these approaches could be used to assess mobility (Sinclair and Boxall 2002b). If these data were supplemented with information arising from fate studies (e.g. degradation route studies and lysimeter investigations) and used in exposure models (FOCUS 2002), it may be possible to derive an estimate of exposure for a transformation product. This could then be used along with the effects estimate to derive a toxicity exposure ratio (TER) (i.e. the ratio of the aquatic ecotoxicity endpoint and the exposure concentration) and hence assess the risk of a particular transformation product.

4.5 Conclusions

In conclusion therefore, there is an increasing need for pragmatic approaches to assess the risks posed to the environment by pesticide transformation products. Generally, transformation products have similar toxicity to or are less toxic than their parent compound. However, in instances where a transformation product is more toxic, the increase in toxicity can be explained by a knowledge of pesticide and transformation product mode of action and the relative accumulation of the transformation product and parent. Using this information, a pragmatic approach has been developed that can be used to assess transformation products at a very early stage in the risk assessment process to identify those products that do and do not need further testing. The use of such an approach offers a range of benefits including cost and time savings and the reduction in animal testing. The

results of the current study are feeding into the EU aquatic ecotoxicology guidance document (European Commission 2002a). Although the current work focuses on the pesticide registration process in Europe, the approach developed here could be adopted by other geographical areas and used with other biologically active molecules (e.g. biocides, human medicines and veterinary medicines). The framework has been evaluated for use in the environmental risk assessment of biocides (Sinclair and Boxall 2002a). Initial results indicate the approach shows promise in this area.

4.5.1 Appendices

Ecotoxicity and physico-chemical property data for parent compounds and associated transformation products collated and utilised during this chapter are available in Table C1 in Appendix C.

5 Prioritization of Transformation Products in Drinking Water Supplies[2]

5.1 Introduction

Pesticide application in agriculture is used to increase crop yield and maintain plant health by eradicating unwanted organisms that compete for resources, bestow disease and/or cause crop damage due to feeding activities. During a normal growing season a wide variety of pesticides can be applied, their identity depends on a range of factors including the specific pest and crop of interest. Once released into the environment, the pesticide is susceptible to biotic and abiotic degradation, which may result in the formation of a range of different transformation products (Roberts 1998; Roberts and Hutson 1999; Aizawa 2001). It is important that during the characterisation of risks posed by pesticides to aquatic ecosystems, the impact of pesticide transformation products is also considered (Belfroid et al. 1998; Kolpin et al. 2001; Fenner et al. 2002; Boxall et al. 2004).

Once formed in the environment, transformation products can move vertically through the soil profile to underlying groundwaters and away from the site of application via aquifer transport (Schiavon 1988; Widmer and Spalding 1995; Broholm et al. 2001). There is also the potential for transformation products to enter surface waters when they travel laterally via either overland runoff due to heavy rainfall or via sub-soil tile drains, entering agricultural ditches and streams and are then transported on to major rivers, reservoirs and ultimately estuaries and the marine environment (Muir and Baker 1976; Phillips et al. 1999; Aga and Thurman 2001). Mobile pesticides and transformation products can be susceptible to degradation at any point during their transport. Mobile and non-mobile transformation products formed from mobile pesticides or transformation

[2] Sinclair C.J., Boxall A.B.A., Parsons S.A., and Thomas, M.R. (2006) Prioritization of Pesticide Environmental Transformation Products in Drinking Water Supplies, Environmental Science and Technology, 40:7283-7289.

products can therefore be identified away from the site of application (Brouwer et al. 1990). Pesticide transformation products have been identified in rivers, reservoirs and groundwater (Albanis and Hela 1998; Kolpin et al. 2000; Battaglin et al. 2000; Mills et al. 2005). There is therefore the potential that raw water abstracted for treatment and subsequent human consumption is contaminated with transformation products and parent pesticides.

Some high profile transformation products, such as deethylatrazine formed from the triazine herbicide atrazine, have been identified in finished drinking waters (Coupe and Blomquist 2004), whilst transformation products of organophosphorus insecticides that have conserved the acetylcholine esterase inhibitory activity of the parent pesticide, a toxic action known to effect human health, have been identified in both raw source water and treated drinking water (EPA 2001b). Moreover chronic effects caused by some transformation products have been identified. The environmental transformation products formed from the chloroacetamide herbicide alachlor have been shown to be more teratogenic than the parent compound (Osano et al. 2002b) and some transformation products have exhibited mutagenic effects (Tessier and Clark 1995). Whilst not all transformation products will exhibit toxicity to mammalian endpoints and even less will exhibit effects greater than their parent pesticide, these examples indicate that the risk of transformation products in source drinking water needs to be considered. There is therefore a need to identify those transformation products that have the greatest potential to reach drinking water supplies and those that are of the greatest concern to human health.

At an American Water Works Association Research Foundation (AwwaRF) workshop (5th June 2004, Prague, Czech Republic), it was agreed that a risk based approach was required by the water industry and pesticide manufacturers. Therefore this chapter describes a simple approach developed to identify pesticide transformation products of potential concern to drinking water supplies. It is envisaged that water companies and water regulators may use the approach to focus future monitoring and water testing programmes. The approach can be

applied to any specific geographical area that has suitable pesticide usage data available. We illustrate the approach with two geographical areas that have suitable data, agricultural pesticide use in Great Britain and agricultural and amenity pesticide use in California which includes use in parks, golf courses, cemeteries, pasture and along roadsides and railways.

5.2 Development of Prioritisation Scheme

5.2.1 Workshop

To aid in the development of a prioritisation scheme for pesticide transformation products, a workshop was organized on 5th June 2004 in Prague, Czech Republic. Thirty scientists with a variety of expertise and backgrounds were brought together to discuss and develop a possible prioritisation scheme. The delegates had experience in environmental fate and effects, pesticide regulation, water treatment, environmental monitoring and analysis, toxicity, ecotoxicity and human health effects. The prioritisation approach described below was developed based on discussions during the workshop.

The impact of a pesticide transformation product on drinking water quality will be determined by 1) its potential to enter drinking water supplies; 2) its treatability and 3) its potential effects on human health. The prioritisation scheme is therefore a risk based approach that considers both exposure and effects. The exposure part of the approach does not predict transformation product concentration in drinking waters but provides a normalised value for the three components used to determine exposure (formation, sorption and degradation). Possible values for each component used to determine exposure can lie between 0 and 1. The approach is therefore designed to rank a transformation product among other transformation products identified within a system.

The extent to which transformation products will be present in finished drinking water will be heavily influenced by the drinking water treatment processes

employed to prepare source water for human consumption. The proposed scheme has been developed so that it is not specific to a particular location and therefore specific treatment processes. Determining the impact of water treatment on transformation products would require data relating to their fate in a range of treatment processes. However, extensive data of this nature is not currently available. Therefore the scheme was restricted to prioritising transformation products in source drinking water and not finished drinking water.

5.2.2 Stage 1: Exposure

The potential for a transformation product to reach drinking water supplies will be determined by a range of factors most notably the amount of parent pesticide used, the scenario in which the parent compound is used, the amount of a particular transformation product formed, the mobility of the transformation product and its persistence in the environment. Therefore in the exposure component of the prioritisation approach the potential for a transformation product to enter drinking water is determined using data on each of these factors.

5.2.2.1 Input into the system

The first action is to define the scope of the prioritisation by identifying the geographical area. This could be a country, an administrative region, an individual catchment or an area determined by other geographical factors such as an area covered by a water company. Once the geographical area (or system) is defined then data from usage surveys can be used to identify the pesticides in use in that area. Using this list of pesticides, their environmental transformation products can be identified from compendia of degradation route studies (Roberts 1998; Roberts and Hutson 1999; Aizawa 2001) along with information on the amounts formed in soil, water and water/sediment degradation studies.

Using the data collected on pesticide usage and transformation product formation an index (A) that reflects the amount of a transformation product that will be released into the system of interest is then calculated using Equation 2.

Equation 2

$$A = \frac{U}{U_{max}} . f$$

Where:

A = Transformation product amount index

U = Total amount of the transformation product's parent pesticide used in the geographical area over a specified time period (e.g. kg yr^{-1})

U_{max} = Total amount of the highest used pesticide in the geographical area over a specified time period (e.g. kg yr^{-1})

f = Maximum fraction of transformation product formed within the environmental compartment of interest

The f value used in the prioritisation should be the maximum fraction of the transformation product formed during a laboratory degradation study. The selection of degradation studies from which the transformation product formation data are drawn will depend on the pesticide usage scenario under investigation. If the prioritisation was for transformation products from agricultural pesticides then formation data from soil and aqueous degradation studies should be considered. However if a scenario where pesticides could directly enter surface waters was under consideration, e.g. hard surfaces, then only aqueous degradation studies should be considered. If several maximum values are collated for a transformation product from degradation studies for the same compartment then the highest identified value should be used to maintain the conservative nature of the scheme.

5.2.2.2 Mobility

Once a transformation product has been formed in the environment, the potential for it to enter and remain in water bodies will be determined by its sorption to soils and/or sediments. The sorptive behaviour of a compound can be described by the distribution coefficient K_d, which is a simple measure of its distribution between the soil/sediment and aqueous phases (Lyman 1995). The sorptive behaviour of a compound is usually influenced by the amount of organic matter present in the soil/sediment (Lambert et al. 1965). Therefore the K_d is often normalized by the amount of organic carbon present in the matrix of interest, yielding the organic carbon normalized adsorption coefficient (K_{oc}). In the second stage of the exposure assessment the mobility index (F) is calculated. This is the fraction of the transformation product that is likely to be in the aqueous compartment of the environment and is therefore likely to enter drinking water supplies. It is determined using Equation 3.

Equation 3

$$F = \frac{1}{1 + K_d r_{sw}}$$

Where:

F =	Mobility index
K_d =	Distribution coefficient for adsorption ($cm^3\ g^{-1}$)
r_{sw} =	Ratio of the aqueous volume and solid phase mass of the compartment of interest

The ability of a transformation product to move to source drinking water will be influenced by its sorptive behaviour, e.g. K_{oc}, and the exposure to sorptive material, i.e. soil and sediment. Transformation products that result from the agricultural application of pesticides will be exposed to more sorptive material than transformation products that are formed as a result of pesticide application to hard surfaces and/or direct application to surface water. Therefore for the agricultural/soil application of pesticides an r_{sw} = 7.5 is proposed (volume

fraction of solids in soil - 0.6 m_{solid}^3 m_{soil}^{-3}, volume fraction of water in soil - 0.2 m_{water}^3 m_{soil}^{-3}, density of the solid phase - 2500 kg_{solid} m_{solid}^{-3}), whilst for applications that do not involve the soil compartment an $r_{sw} = 0.005$ is proposed (volume fraction of solids in sediment - 0.2 m_{solid}^3 $m_{sed.}^{-3}$, volume fraction of water in sediment - 0.8 m_{water}^3 $m_{sed.}^{-3}$, density of the solid phase - 2500 kg_{solid} m_{solid}^{-3}, depth of water in surface water body - 3m and depth of sediment in that surface water - 0.03m). These values are from the standard environmental characteristics proposed in the European Chemicals Bureau Technical Guidance Document on Risk Assessment (TGD) (ECB 2003). Within the available literature, transformation product sorption data are often reported as K_{oc} and not as K_d. Moreover, K_{oc} values are often reported without the total organic carbon content (TOC) of the soil in which the determination was made. Therefore, if this is the case, a TOC of 2% for the soil/sediment was assumed to derive K_d, again this value having been proposed in the TGD (ECB 2003).

5.2.2.3 Persistence

Once formed in the environment the potential for a transformation product to enter drinking water supplies will depend on the time the compound remains in the environment. The persistence of the compound in the environment will be determined by how susceptible it is to biotic and abiotic degradation. In the third phase of the exposure assessment, a persistence index (*P*) is therefore determined using Equation 4. When characterizing the environmental persistence of transformation products, a compound's degradation rate constant in both the soil and water compartments will significantly influence the overall persistence and hence the potential to enter source drinking waters. Therefore the persistence index is derived from degradation half-lives for both compartments. The two factors assume that degradation follows first order kinetics and calculate the fractions remaining in both compartments after a designated period of time, which are then multiplied to provide the overall persistence index. Potential values for this index range from 0 to 1.

Equation 4

$$P = e^{-\frac{\ln 2}{DT_{50w}}.t} . e^{-\frac{\ln 2}{DT_{50s}}.t}$$

Where

P =	Persistence index
$DT_{50\,w}$ =	The time for 50% of a transformation product to be reduced in an aqueous degradation study (days)
$DT_{50\,s}$ =	The half time for 50% of a transformation product to be reduced in a soil degradation study (days)
t =	Residence time of water in the system (days)

Pesticide transformation product degradation half-lives are often available for different environmental compartments, e.g. soil and sediment/water systems and different degradation processes, e.g. hydrolysis and surface photolysis. When prioritising transformation products resulting from the agricultural application of pesticides then the determination of P should include degradation rate constants in both soil and water (Equation 4). Where pesticides are applied directly to surface waters and/or used on hard surfaces, then only the water persistance component ($DT_{50\,w}$) should be used to determine P in Equation 4 because the degradation rate constants in soils will not influence the environmental fate of these transformation products. When selecting a water degradation half-life to calculate P, the lowest value from either a hydrolysis study, aqueous photolysis study or a sediment/water degradation study should be used, as it will be this process that drives the degradation of the transformation product in water. The TGD (ECB 2003) water residence value of 40 days is suggested for use as the t parameter. However it may be required to alter this value depending on the drinking water source under consideration, e.g. for drinking water sourced primarily from groundwater this value may need to be increased.

5.2.2.4 Calculation of the Exposure Index

The three previously described parameters; formation, mobility and persistence, are multiplied in the final stage of the exposure assessment to provide a single

index for exposure (E) using Equation 5. E is a unitless value that allows a transformation product to be ranked on its potential to enter drinking water supplies relative to the other transformation products that could be formed within the system of interest.

Equation 5 $$E = A.F.P$$

Where

E = Transformation product exposure index

5.2.3 Stage 2: Effects

Limited data are available on the mammalian and human health toxicity of pesticide transformation products (Parsons et al. 2006). Therefore in the absence of suitable information, the potential health effects of the associated parent compound should be used in the effects component of the prioritisation exercise. Parent compounds are generally more toxic than transformation products (Heydens et al. 2000; Sinclair and Boxall 2003) and so the use of parent pesticide data is likely to be conservative. The most relevant toxicological safety value for drinking water is the acceptable daily intake (ADI). These values are therefore used in the prioritisation approach. ADIs are usually calculated for risk assessment, generally by extrapolating the lowest no-observable effect level (NOEL) identified during mammalian toxicity studies to humans with the use of a safety factor, which is often 100. Many governments and organizations have adopted this approach so that there can be several ADIs available for any pesticide. If available then the ADI for the specific jurisdiction should be used, however if this is not available then to err on the conservative side, the lowest ADI identified should be used in the prioritisation scheme.

5.2.4 Stage 3: Risk characterization and ranking

In the final stage of the prioritisation, a risk index (*RI*) is derived from the transformation product exposure index and the parent ADI using Equation 6. The larger the *RI* the greater the potential risk posed by a transformation product to drinking water supplies within the defined system. By ranking each transformation product formed in a study system according to its *RI*, it is possible to identify those substances that pose the greatest risk to drinking water supplies. This information can then be used to steer future monitoring and research.

Equation 6

$$RI = \frac{E}{ADI}$$

Where

RI = Transformation product risk index

ADI = Acceptable daily intake (mg kg^{-1} day^{-1})

When the same transformation products are produced from different parents, e.g. deisopropylatrazine is a product of both atrazine and simazine then the *RI* should be summed to provide an *RI* that represents the overall risk posed by that transformation product within the system of interest.

5.2.5 Input data and data gaps

In order to complete a priority list, once a system has been defined, it may be necessary to use transformation product data from a variety of sources, e.g. experimentally determined data and/or default values. The quality and accuracy of the data used to generate a priority list can vary. Therefore it is suggested that transformation products should be classified by the quality of the data used, grouped according to these classifications and only then be ranked according to their *RI*. A proposed classification system is provided in Table 15. This

grouping allows those transformation products that have been prioritised based on potentially less accurate data to be distinguished from those transformation products with good quality datasets. The *RI* for transformation products that are categorized as Class A can be considered a representation of the risks posed by these compounds compared to the other transformation products in that class. Transformation products that have a *RI* generated using four default values, i.e. Class E should be omitted from a final priority listing until some experimentally derived data becomes available.

Table 15. Categories to be used when classifying the transformation product data availability

Data class	Default values required [a, c]
A	0
B_f	1 (formation) [b]
B_m	1 (mobility)
B_p	1 (persistence)
C	2
D	3
E	4

[a] - There are four parameters in the classification: *f*, K_d, $DT_{50\,s}$ *and* $DT_{50\,w}$

[b] - Transformation product formation data in the form of minor/major should be considered as default data

[c] - The subscript *f*, *m* and *p* on the B data class represent the single default value data type required in the prioritisation was for formation, mobility or persistence respectively

5.2.6 Priority list for California and Great Britain

To illustrate the proposed approach two priority lists were developed: 1) agricultural pesticide use in Great Britain and 2) agricultural and amenity pesticide use in California, USA.

A pesticide usage dataset compiled by the Pesticide Usage Survey Group (PUSG) of the Central Science Laboratory was used to define the scope of the Great Britain priority list. The PUSG undertakes surveys of all crops grown commercially throughout the UK at regular intervals, using fully stratified samples of farmers and growers. The data are then extrapolated to provide a national estimate of use (Thomas 2001). The dataset used during this

prioritisation comprised 'field' pesticide usage in Great Britain during 2003. These data did not include pesticides applied during food storage practices and pesticide applications under covered scenarios such as glasshouses and mushroom production.

The California Department of Pesticide Regulation (CDPR) carries out a comprehensive program for monitoring pesticide usage throughout the state. Under this program all pesticide usage has to be reported on a monthly basis. This data includes the date of application, the location of application, pesticide identity and quantity used (CDPR 2000). The pesticide usage data used for California was defined as 'agricultural' but also included applications to parks, golf courses, cemeteries, pasture, and along roadsides and railways. The usage data excludes home and garden use and most industrial and institutional use (CDPR 2000). The dataset used during this prioritisation comprised pesticide usage during 2003 (CDPR 2005).

Principally, data for the generation of priority lists for Great Britain and California were obtained from regulatory documents. Where no regulatory data were available, data were obtained by searching the publicly available literature (Parsons et al. 2006). If no experimentally determined data could be identified, conservative default values were used (Table 16). When several data values and/or ranges of values had been collated for a given transformation product then the most conservative value was used during the prioritisation. Where an information source provided reported data as less than a specified value, e.g. <5%, the specified value was used in the prioritisation and this value was not classified as a default value.

Table 16. Proposed conservative default values to be used during a transformation product prioritisation when experimental data are unavailable

Parameter	Collated value	Proposed default value	Units
f	-	1	-
f	minor	0.1	-
f	major	1	-
f	< X%	X / 100 [b]	-
f	> X%	1	-
K_d	-	0.2 [a]	$cm^3 g^{-1}$
$DT_{50\,s}$ and $DT_{50\,w}$	-	300 [a]	days

[a] - conservative default values derived from ECB (2003)

[b] - For example if available formation data was, < 8%, f = 0.08

5.3 Results and Discussion

The dataset used to illustrate the prioritisation scheme for agricultural pesticide use in Great Britain contained 227 compounds which had annual usage greater than 500 kg. Those compounds that were considered to be inorganic, e.g. sulphur and/or had an undefined chemistry, e.g. tar oil were removed (n = 11). Sixteen of the remaining pesticides were characterised within the literature as having no environmental transformation products, whilst 23 pesticides had transformation products identified but no environmental formation data available and were therefore excluded from the list (the illustration was restricted to transformation products with quantitative or qualitative formation data) (Table D1 in Appendix D). No environmental transformation products could be identified for 55 of the pesticides, however, 371 transformation products with environmental formation data were identified for the remaining 122 pesticides. The top four transformation products with data availability categorised as Class A, B_f, B_m, B_p, C and D for agricultural pesticide usage in Great Britain are provided in Table 17. When the priority list for Great Britain was compiled, approximately 74% of the identified transformation products required three or more default values (Class D and E), with only 12 compounds (3%) having a complete dataset.

Table 17. Priority list of transformation products in Great British drinking water supplies as a result of pesticide application

Transformation product	Parent pesticide(s)	Pesticide usage (*U*) (kg yr^{-1})	Formation fraction (*f*)	Sorption (K_d) (cm^3 g^{-1})	Persistence soil ($DT_{50\,s}$) (d)	Persistence water ($DT_{50\,w}$) (d)	Data availability classification	Pesticide ADI (mg kg^{-1} d^{-1})	Risk index
3,5,6-trichloro-2-pyridinol	chlorpyrifos / triclopyr	67684 / 38295	0.32 / 0.26	0.53	279	383	A	0.003 / 0.005	0.69
thifensulfuron acid	thifensulfuron-methyl	16786	0.25	0.138	365	109	A	0.01	0.066
kresoxim-methyl acid	kresoxim-methyl	94944	0.84	0.34	131	383	A	0.4	0.019
O-desmethyl thifensulfuron-methyl	thifensulfuron-methyl	16786	0.19	0.68	15.3	51	A	0.01	0.002
CGA-321113	trifloxystrobin	76011	1	0.96	350	289	Bf	0.038	0.091
carbendazim	thiophanate-methyl / benomyl	18633 / 922	0.76 / 1	0.45	320	743	Bf [a]	0.02 / 0.03	0.066
1,2,4-triazole	fluquinconazole / tebuconazole tetraconazole / propiconazole myclobutanil	22443 / 126787 4906 / 10760 3877	0.161 / 0.06 0.1 / 0.43 1	0.86	98	190	Bf [a]	0.006 / 0.03 0.004 / 0.04 0.1	0.044
CL 153815	picolinafen	3103	1	3.2	77	31.4	Bf	0.014	0.001
diclofop acid	diclofop-methyl	33683	0.9	0.2	63	105	B_m	0.001	2.653
ethyl-m-hydroxyphenyl carbamate	desmedipham	4349	0.16	0.2	27	26	B_m	0.0018	0.008
triazine amine A	tribenuron-methyl	4074	0.91	0.2	240	105	B_m	0.12	0.004
BTS 27919	amitraz	642	0.35	0.2	150	21	B_m	0.0025	0.004
desmethylisoptoturon	isoproturon	2260278	0.14	1.07	65	300	Bp	0.015	0.615
deethylatrazine	atrazine	139758	0.19	1.7	121	300	Bp	0.006	0.277
deisopropylatrazine	simazine / atrazine	139758	0.11 / 0.1	0.16	17	300	Bp	0.005 / 0.006	0.201
thiophene sulfonimide	thifensulfuron-methyl	16786	0.29	0.052	96.6	300	Bp	0.01	0.106
propachlor oxanilic acid	propachlor	138592	0.33	0.03	300	300	C	0.009	1.539
propachlor ethane sulfonic acid	propachlor	138592	0.19	0.03	300	300	C	0.009	0.883
4-hydroxy-2,5,6-trichloroisophthalonitrile	chlorothalonil	479833	0.32	0.2	43	300	C	0.018	0.722
triazamate metabolite II	triazamate	1020	0.91	0.28	300	300	C	0.0003	0.367
1-methyl-3-(4-isopropyl phenyl)-urea	isoproturon	2260278	0.16	0.2	300	300	D	0.015	3.458
TCPSA	tri-allate	372093	0.18	0.2	300	300	D	0.005	1.916
3-carbamyl-2,4,5-trichlorobenzoic acid	chlorothalonil	479833	0.25	0.2	300	300	D	0.018	0.98
methiocarb sulfoxide	methiocarb	38567	0.3	0.2	300	300	D	0.002	0.851

[a] - B_f represents the lowest data availability classification received by 1,2,4-triazole and carbendazim

The dataset used for the prioritisation of transformation products from pesticide usage in California contained 100 of the most used compounds (by mass) during 2003. Those compounds that were considered to be inorganic, e.g. sulphur, had an undefined chemistry, e.g. petroleum oil and/or were known pesticide adjuvants were removed (n = 41). The prioritisation was then undertaken on the remaining 56 compounds. Eighty-six transformation products were identified from 33 pesticides, the remaining 24 pesticides were either characterised within the literature as having no environmental transformation products or no data were available on their environmental degradation (Table D2 in Appendix D). The top four transformation products with data availability categorised as Class A, B_p, C and D for agricultural and amenity pesticide usage in California are provided in Table 18 (no transformation products were classified as B_f or B_m). Approximately 70% of the transformation products identified for California required three or more default values (Class D and E) to complete the prioritisation, with only 4 transformation products (5%) having a complete dataset.

Table 18. Priority list of transformation products in California drinking water supplies as a result of pesticide application

Transformation product	Parent pesticide(s)	Pesticide usage (U) (kg yr^{-1})	Formation fraction (f)	Sorption (K_d) (cm^3 g^{-1})	Persistence soil ($DT_{50\,s}$) (d)	Persistence water ($DT_{50\,w}$) (d)	Data availability classification [a]	Pesticide ADI (mg kg^{-1} d^{-1})	Risk index
carbendazim	thiophanate-methyl	57118	0.76	0.45	320	61	A	0.02	0.08
aldicarb sulfoxide	aldicarb	118887	0.92	0.17	53	2.3	A	0.003	<0.001
RP 30228	iprodione	130467	0.31	132	319	1.8	A	0.02	<0.001
aldicarb sulfone	aldicarb	118887	0.8	0.09	154	0.9	A	0.003	<0.001
3,5,6-trichloro-2-pyridinol	chlorpyrifos	701468	0.32	0.53	279	300	Bp	0.003	3.549
tetrahydrophthalamide	captan	226783	0.66	0.04	19.5	300	Bp	0.1	0.043
aminomethylphosphonic acid	glyphosate	2702064	0.29	15	958	300	Bp	0.3	0.007
3-phenoxybenzoic acid	cypermethrin	84414	0.48	1.46	300	3	Bp	0.015	<0.001
methylisothiocyanate	metam-sodium	6720247	0.75	0.2	10	300	C	0.01	2.671
N'-(3,4-dichlorophenyl)-N-methylurea	diuron	609442	0.23	0.2	1733	300	C	0.007	1.635
deisopropylatrazine	simazine	305784	0.11	0.16	300	300	C	0.005	0.557
malathion dicarboxylic acid	malathion	296716	0.62	0.2	300	365	C	0.05	0.289
pyrimidinol	diazinon	237584	0.73	0.2	300	300	D	0.002	6.695
3,5,6-trichloro-2-methoxypyridine	chlorpyrifos	701468	0.08	0.2	300	300	D	0.003	1.446
2-hydroxy ethyl phosphonic acid	ethephon	260529	0.64	0.2	300	300	D	0.018	0.711
1-napthol	carbaryl	93022	1	0.2	15	300	D	0.003	0.41

[a] - No transformation products were classified as B_m and B_f

If a prioritisation were to be used to focus monitoring studies on the highest risk transformation products then compounds that are present at the top of the separate data classes (Class A, B_f, B_m, B_p and C) may be selected. These compounds could be considered as those that would pose the greatest risk to drinking water resources within a system, based on currently available data. Generally, the identity of the transformation products ranked at the top of each data availability classification are different for Great Britain and California. Therefore it may not be appropriate to use standard transformation product determinand lists when monitoring surface water and groundwaters. It is difficult to compare surface and groundwater transformation product monitoring data to the generated priority lists because data specific to the defined systems are not available. However when we consider the top of the priority lists for Great Britain and California (Table D3 and D4 in Appendix D, respectively) a number of the transformation products have previously been identified in surface and groundwater (Sinclair and Boxall 2005), e.g. 3,5,6-trichloro-2-pyridinol, deisopropylatrazine and deethylatrazine.

The aim of this study was to develop a prioritisation scheme that could be used as a tool to allow the water industry and regulators to focus future research and monitoring towards those pesticide transformation products of most importance in terms of their tendency to entering drinking water supplies and to negatively affect human health. The approach can be applied to different geographical areas where suitable pesticide usage data are available. The approach was not devised to provide estimated concentrations of transformation products in environmental waters or determine whether individual transformation products will be present in drinking water supplies, but to rank the potential for pesticide transformation products to enter drinking water supplies in relation to other transformation products present within a specified system of interest, i.e. geographical area or specific use scenario. It is important to recognize that the approach has been developed for ranking purposes only and a high *RI* does not indicate that a substance actually poses an unacceptable risk to human health but that it may pose a higher risk than other transformation products in that system.

A number of approaches have previously been derived to assist in the identification of pesticides, veterinary medicines and other persistent, bioaccumulative and toxic chemicals (Mitchell et al. 2002; Boxall et al. 2003) that are of most concern in terms of their impact to environmental ecosystems (Russom et al. 1995). These methodologies generally consider the risk of parent compounds in terms of their impact to the environment and not human health. Due to the lack of available data within the open literature it has been difficult to draw any conclusions upon the risk of pesticide transformation products (Belfroid et al. 1998). Moreover some of the approaches developed for characterising risk are very data intensive, incorporating physico-chemical properties, site specific parameters and mammalian toxicity endpoints (Enfield et al. 1982; Rao et al. 1985; Capleton et al. 2006). Techniques of this nature maybe useful for determining the most important well known chemicals at well-characterised sites but it would be difficult to apply them to larger, generally uncharacterised geographical areas and extensive transformation product inventories.

The environmental fate and effects data availability for pesticide transformation products severely hampers the generation of a complete priority list once pesticide usage data has been identified. Russom et al. (1995) acknowledged that environmental screening methodologies for pesticides were restricted by the availability of suitable exposure and effects data. Therefore they developed an approach that used quantitative structure activity relationships (QSAR) to fill ecotoxicological data gaps, quantitative structure biodegrability relationships (QSBR) to determine persistence and fugacity models to estimate partitioning. The use of relatively accurate estimated values for persistence and mobility would allow compounds to be placed realistically during a prioritisation. The more default values that are used for a transformation product then the larger the allocated *RI*, due to the conservative nature of these values. In this scheme a default of 300 days for $DT_{50\,s}$ and $DT_{50\,w}$ was proposed, as suggested by the EC (European Commission 2002a). This value, when compared to experimentally

derived data is rather conservative, 88% of transformation products have a $DT_{50\,s}$ less than this value, with 42% having a $DT_{50\,s}$ an order of magnitude less than this value (Sinclair and Boxall 2005). However, if predictive values were to replace conservative default values, there is a requirement to identify the most suitable techniques to use for this purpose.

Due to the very limited availability of mammalian and human effects data, parent pesticide ADIs were used for the hazard input within the prioritisation scheme. These data are probably very conservative, however it is probable that pesticides that are toxic to humans are more likely to degrade to transformation products that are toxic to humans, than pesticides that are not toxic to humans, i.e. if a structural moiety which infers a specific toxic action is maintained within a transformation product there is the possibility that the transformation product will exhibit the same toxic mechanism as the parent. Currently there is a trend to reduce the number of mammalian toxicity studies that are performed and identify suitable alternative methodologies (ECVAM 2006). Expert methods that identify structural alerts that may cause molecules to exhibit known toxicological mechanisms, e.g. DEREK for Windows (Lhasa Ltd), could be used to provide transformation product specific toxicological data for future prioritisations.

5.4 Conclusions

The advantages of the proposed scheme are that transformation products identified within a system of interest can be rapidly ranked in terms of their risk to drinking water supplies. This information could be invaluable in prioritising chemicals for analytical method development, monitoring programs and experimental toxicology and ecotoxicological studies. The approach could be expanded in the future to include predictive toxicological and environmental parameter approaches that could negate the requirement for conservative default values and thereby refine priority lists for pesticide transformation products.

5.4.1 Appendices

Supporting information are available in Appendix D: Details of the pesticides eliminated from the Great Britain and California prioritisations and the reasoning for their omission (Table D1 and D2 respectively), all transformation products considered and their risk index for the Great Britain and California prioritisations (Table D3 and D4 respectively) and calculated indices (*A*, *F*, *P*, *E* and *RI*) for the top four transformation products from each illustrative example (Table D5).

6 The Consideration of Environmental Pesticide Transformation Product Mammalian Toxicity for Use in Risk-Based Human Health Prioritisations

6.1 Introduction

Following release to the environment, pesticides may remain at the site of application, move laterally to surface waters, vertically to groundwater or succumb to biotic or abiotic degradation. The breakdown process can form transformation products that maybe more mobile and/or more persistent than their parent pesticide and are therefore regularly detected more frequently and at higher concentrations in surface and groundwaters than their parent pesticides (Kolpin et al. 2000). Those formed from herbicides, such as atrazine and glyphosate, are commonly found in environmental waters in Europe (Skark et al. 1998; Albanis et al. 1998) and North America (Kolpin et al. 1997; Wan et al. 2006), whilst the detection of insecticidal and fungicidal transformation products are reported less frequently. Within an individual catchment >350 transformation products may be formed from the pesticides applied (Sinclair et al. 2006), however only very few of these compounds are regularly monitored for in surface and groundwaters (Gilliom et al. 2006) and recently transformation products from intensively used herbicides have been detected in finished drinking waters up to 1.5μg/L (Hladik et al. 2006), so there is potential for consumer exposure.

Within the environment the majority of transformation products exhibit reduced ecotoxicity to non-target aquatic organisms when compared to their parent pesticides, however some can be more potent (e.g. Stratton and Corke 1982; Osano et al. 2002b), with increased potency attributed to changes in accumulation and mode of action or maintenance of the toxicophore allowing exhibition of the parental mode of action (Sinclair and Boxall 2003).

Detrimental environmental effects caused by pesticide transformation products are not a recent phenomenon, some of the most publicised impacts of pesticides on non-target organisms in the past have been a result of transformation products rather than parent pesticides. For example, egg shell thinning in wild birds was attributed to 1,1-dichloro-2,2-bis(4-chlorophenyl)ethylene (DDE), a primary transformation product of the organochlorine insecticide DDT (Blus et al. 1971). In comparison to the ecotoxicological effects to non-target organisms, data availability on the toxicological effects of transformation products to mammals is relatively limited. However some transformation products have demonstrated mutagenicity (Tessier and Clark 1995; Matsushuta et al. 2002) and estrogenic activity (Kelce et al. 1995; Gaido et al. 1999).

In the absence of experimental data, predictive toxicological techniques are often used to identify the most potentially harmful chemicals so that experimental resources can be exploited most effectively (Russom et al. 1995; Chaudhry et al. 2006). Previously in Chapter 5, transformation product risk characterisation for drinking water consumers has used parent pesticide acceptable daily intake values (ADI) as a surrogate for transformation product toxicological data (Sinclair et al. 2006). Whilst surrogate data are suggested to fill data gaps (Swanson and Socha 1997), it is anticipated that transformation product toxicity will be over estimated in the majority of cases but sometimes could be under estimated. Therefore due to a general absence of experimental toxicological data for most transformation products that may be formed in the environment, the aims of this study were to 1) Explore the relationships between available experimentally derived transformation product and parent toxicological data; 2) Evaluate models that could be used in the absence of experimental data; and 3) Undertake a case study to illustrate how transformation products specific toxicological data can be combined with exposure methods to identify those compounds of most concern.

6.2 Materials and Methods

6.2.1 Experimentally determined transformation product toxicity

Experimental data were collated on transformation product and parent pesticide toxicity from a number of sources (EPA 2007; PSD 2007; EU 2007b; EU 2007b; PMRA 2007c; EFSA 2007e). Collection focussed on the most frequently reported endpoints, mutagenic/genotoxic potential and rat oral LD_{50}. The available data on the mutagenic potential of transformation products are inconsistent, therefore three groups of data types were identified; 1) result of the Ames test is specified, e.g. 'Ames test negative', 2) result of a test which refers to a bacterial and/or gene reversion assay but does not specify the Ames test, e.g. 'in-vitro bacterial gene mutation negative' and 3) result reports general mutagenic/genotoxic potential, e.g. 'no mutagenic activity'. Collated transformation product and respective parent pesticide mutagenic and rat oral LD_{50} toxicological data were compared.

6.2.2 Evaluation of predictive methodologies

Collated transformation product experimental mutagenic and rat oral LD_{50} data were used to evaluate the predictive ability of two commonly used predictive toxicological approaches, namely DEREK for Windows version 9.0.0 (Lhasa Ltd.) (Sanderson and Earnshaw 1991) and TOPKAT version 6.2 (Accelrys Inc.) (Enslein 1988; Enslein et al. 1994). DEREK attempts to match structural alerts to the structure of query molecules and then provides a qualitative likelihood of the query compound exhibiting the toxicity linked to the matched alert, with likelihoods ranging from 'certain' to 'impossible'. The structural alerts are a 'set of structural features' in a molecule that would allow an expert toxicologist to suggest that a compound may exhibit a particular toxic effect (Anon. 2005). TOPKAT contains multivariate statistical relationships to estimate a range of toxicological (and ecotoxicological) endpoints. Chemical descriptors used to quantify chemical transport properties and the biochemical interaction with the

target site are derived from query molecules and then used within the relationships to provide quantitative or probabilistic estimates. TOPKAT also provides the user with a measure of whether a query compound fits within the predictive domain of the model, termed 'optimum prediction space' by TOPKAT which is a multivariate descriptor space (Anon. 2004).

Transformation product structures were drawn in ChemDraw Ultra version 10.0 (CambridgeSoft Corporation) and saved as '.cdx' files. SMILES notation (Weininger 1988) were produced using the 'convert to SMILES' function in the Excel version 9.0 (Microsoft Corporation) add-on, Accord for Excel version 6.1 (Accelrys Software Inc.). Mol files were produced by converting '.cdx' files to '.mol' files using ISIS/Draw version 2.5 (MDL Information Systems Inc.).

6.2.3 Predictive interpretation

TOPKAT provides the user with a quantitative estimate of toxicity, e.g. rat oral LD_{50} in mg kg^{-1} body weight or a probability that the query compound would produce a positive response in an experimental assay (Enslein et al. 1994). Following standard interpretation (Cariello et al. 2002; Anon. 2004), if probabilities were >70% then the compound was considered likely to produce a positive response, whilst if the probability was <30% then the compound was considered unlikely to produce a positive response. If TOPKAT probabilities were between these two values then this was considered too near to chance (50%) and it was acknowledged that the software could not provide a meaningful (indeterminate) estimate for that endpoint (Anon. 2004). TOPKAT predictions were only used if they fell within the optimum prediction space or they fell outside the optimum prediction space but within a permissible range (as determined by TOPKAT). Results were not considered for end-points were the program identified that a prediction may be unreliable because either 1) the prediction was outside the optimum prediction space and outside the permissible range or 2) the prediction was outside the optimum prediction space and within

the permissible range but a structural fragment from the query compound was not represented in the training set of the model.

DEREK does not provide a probability or a quantitative estimate for a query compound but identifies whether specific structural alerts, i.e. sub-structural moieties linked to specific end-points, are present within the query molecule and also provides the user with a qualitative indication of the potential for the compound to exhibit that end-point. Therefore DEREK estimations were considered to provide a positive response for an end-point when an alert for that end-point was identified within a query molecule and that estimate was categorised as at least 'plausible'. DEREK was assumed to provide a negative response for the end-point of interest if no structural alerts for that end-point were identified.

6.3 Results and Discussion

6.3.1 Comparison of pesticide and transformation product toxicity

During data collation, the mutagenic/genotoxic potential of 149 transformation products was collated, 116 of which had their chemical structure identified. Rat oral LD_{50} data were collated for 153 transformation products with chemical structure identified for 115, 106 transformation products had data available for both toxicological end-points. There was a tendency for pesticide and transformation product rat oral lethal dose data to be reported as an inequality, e.g. >5000 mg kg^{-1} body weight, with only 49 comparisons (32%) between parent and transformation product reported with both values as exact numerics. The majority of these transformation products (71%) were within an order of magnitude of parent pesticide lethal dose values (Figure 20).

Nine transformation products were more than an order of magnitude more toxic than the respective parent pesticide, with most attributed to a comparison with

parental insecticides that require activation to exhibit acetylcholinesterase inhibition. These included the active transformation product carbofuran and its primary degradate 3-hydroxycarbofuran both formed from carbamate pro-insecticides, benfuracarb and carbosulfan, the active cholinesterase inhibitor omethoate formed from the phosphorothiolothionate organophosphorus insecticide dimethoate (Copping and Hewitt 1998; Roberts and Hutson 1999) and three transformation products formed from the organophosphorus insecticide diazinon, S,S-TEPP, O,S-TEPP and TEPP. These are at least two orders of magnitude more toxic than diazinon which requires metabolism to diazoxon to become active and whilst this occurs when dosing rats, a number of additional major metabolites are also formed, thereby reducing the effective dose (Roberts and Hutson 1999). Distinct from this insecticidal trend is the transformation product RPA 412708, formed from the imidazolinone fungicide fenamidone (Tomlin 2006).

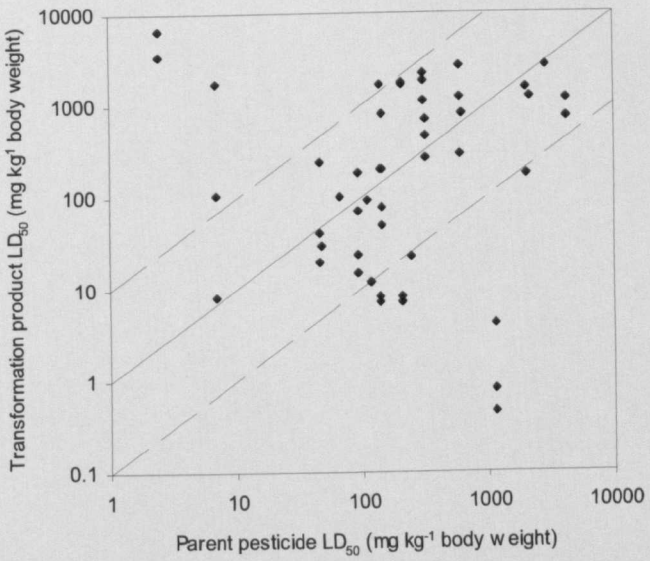

Figure 20. Comparison of pesticide and transformation product rat oral LD_{50} values (where both values are reported as numerics) (solid line x=y, hashed lines equal one order of magnitude more or less toxic)

When all LD_{50} pesticide and transformation product comparative data were analysed in a qualitative manner, including data reported as an inequality, by comparing their allocated class according to the Hodge and Sterner scale (Hodge and Sterner 1949), 51 transformation products (33%) were allocated to a more toxic class than their parent pesticide with eleven of those (which included the three diazinon transformation products) allocated to toxicity classes two or more classes, more toxic than their parent pesticide (Table 19).

Table 19. The comparative classification of rat oral LD_{50} values for transformation products and their respective parent pesticides, occasions where a transformation product was allocated to a more toxic class than the parent pesticide are in bold

		Transformation products				
	Toxicity class [a]	extremely high toxicity	high toxicity	moderate toxicity	low toxicity	very low toxicity
Pesticides	extremely high toxicity	-	-	-	-	-
	high toxicity	-	7	3	5	1
	moderate toxicity	-	**9**	10	18	4
	low toxicity	**2**	**1**	**3**	25	3
	very low toxicity	-	-	**8**	**28**	26

[a] - The Hodge and Sterner class 'relatively harmless' is not provided within the table since no pesticide or transformation product was allocated to that class

When mutagenicity was considered the majority (86.6%) of transformation products demonstrated no reported mutagenic/genotoxic potential. The remaining 20 compounds produced a positive result in one or more mutagenicity studies. Eleven of those were formed from parent pesticides that exhibit a potential for mutagenicity and nine were formed from pesticides with no reported genotoxic potential. Again activation of benfuracarb and carbosulfan produced transformation products, carbofuran and 3-hydroxycarbofuran, that exhibit a toxicity not present in their pre-cursor, whilst the other transformation products that exhibited mutagenicity, reportedly absent from their parent pesticide were KIF-230-M4 formed from the fungicide benthiavalicarb, three transformation products of the fungicide mepanipyrim and phenoxazone formed from the insecticide phosalone.

Whilst it is indisputable that some transformation products exhibit increased mammalian toxicity compared to their parent pesticide, the extent demonstrated here is probably skewed towards over exhibition of this tendency. Toxicological studies are not performed lightly, particularly with a desire to reduce unnecessary animal testing. It is therefore probable that studies reported within pesticide evaluation summary documents, used in this study, will tend to have been triggered and performed when a potential hazard had been identified, maybe due to its structure, the potency of its parent pesticide or maybe its own potency in other studies, e.g. ecotoxicological. Toxicological studies are therefore not routinely undertaken for all transformation products thereby skewing the results of this analysis towards those that are most likely to pose a hazard.

6.3.2 Evaluation of predictive approaches

Evaluation of predictive ability was only possible for transformation products where molecular structure could be determined since this was the required input parameter for both evaluated methods.

6.3.2.1 Mutagenic potential

93% of non-mutagenic transformation products had no mutagenic alerts identified in their structure by DEREK, with only 7 compounds identified as false positives (<7%). Eighteen transformation products have experimental data that indicate they will exhibit mutagenic potential, of these only three were correctly estimated by DEREK to be mutagens by highlighting a structural alert for mutagenesis in their structure. Therefore 15 mutagenic transformation products had no mutagenic structural alerts identified and can therefore be considered false negatives (Table 20).

TOPKAT was unable to provide an estimate for four transformation products due to structural parameterisation problems, whilst 4 compounds were allocated an indeterminate probability for mutagenicity and 27 compounds were estimated to be outside the optimum prediction space and the optimum prediction space

limits of the model(s). When the three types of mutagenic data were considered by TOPKAT, 56% of the non-mutagenic compounds were estimated as non-mutagens and 12 compounds identified as false positives. If compounds with a valid estimate were considered, i.e. not indeterminate, and were within the applicability domain of TOPKAT, the predictive ability for correctly identifying non-mutagens increased to 83%. TOPKAT correctly identified two mutagenic transformation products as mutagens whilst thirteen were estimated to be non-mutagens, i.e. false negatives (Table 20).

Table 20. The predictive ability of DEREK and TOPKAT to estimate mutagenicity for pesticide transformation products

Date type	Experimental		DEREK		TOPKAT			
			concordant	discordant	concordant	discordant	indeterminate	OOPS[b]
Ames test	-'ve	67	63	4	43	5	0	19
	+'ve	8	0	8	1	7	0	0
Bacterial/gene reversion	-'ve	9	8	1	5	3	0	1
	+'ve	4	0	4	0	3	1	0
General mutagenic/ genotoxic potential	-'ve	26[a]	24	2	9	4	2	7
	+'ve	6	3	3	1	3	1	1
Overall	-'ve	102	95	7	57	12	2	26
	+'ve	18	3	15	2	13	2	1

[a] - TOPKAT was unable to process four transformation products in the -'ve general mutagenic/genotoxic potential class
[b] - Outside optimum prediction space and optimum prediction space limits

Prior to this study no techniques had been evaluated for their ability to estimate mammalian end-points specifically for pesticide transformation products. However, DEREK and TOPKAT have been evaluated for their ability to estimate mutagenicity for a number of other chemical classes. TOPKAT performed better than DEREK when evaluated for their ability to correctly predict whether pharmaceuticals would produce positive or negative responses in a bacterial mutagenicity assay, 73% of molecules were correctly classified as either mutagens or non-mutagens. Importantly, TOPKAT generated more false negatives for actual mutagens than DEREK, with 60% of the compounds known to produce positive results in a mutagenic assay estimated as non-mutagens, whilst DEREK only fared slightly better with 54% (Cariello et al. 2002). During

a similar evaluation of 100 structurally diverse chemicals, the overall predictive ability of TOPKAT was similar (74%), whilst the ability to correctly allocate these chemicals as mutagens was substantially better (71% against 40%) (Zeiger et al. 1996). During this study DEREK correctly classified 82% correctly as mutagens or non-mutagens whilst the TOPKAT performance was lower (49%) since 26% of compounds where outside the domain of the model or were provided an indeterminate estimate. The increased overall performance of DEREK could be attributed to the bias within the transformation product dataset for non-mutagens since only 17% of mutagens were estimated correctly.

DEREK and TOPKAT have demonstrated a better predictive ability when correctly categorising pharmaceutical mutagens that contained the 'Ashby carcinogenic alerts' (Ashby and Tennant 1991) (83% and 73% respectively) than those without obvious structural alerts (27% and 18% respectively) (Snyder et al. 2004). Whilst the mutagenic predictive ability can vary depending on chemical type and/or moieties present, it has been suggested that since SAR based approaches, such as TOPKAT, do not use presumed mechanisms of action then their ability to predict other effects such as carcinogenicity will be similar to their ability to estimate mutagenicity. However it would be difficult for any predictive approach to achieve 100% concordance with experimentally determined mutagenic potential when inter- and intra- laboratory reproducibility for these studies can only produce positive and negative concordance of 85% (Zeiger et al. 1996). Therefore it is unfair to expect models to fair better than the reproducibility of the end-point they attempt to predict. The previous evaluations of TOPKAT and DEREK were undertaken using earlier versions of the programs, therefore it is difficult to make exact comparisons between their ability to estimate the toxicity of pharmaceuticals, industrial chemicals and transformation products since it may be a differences in the programs themselves rather than an actual perceived ability to perform better estimating toxicity for a certain group of chemicals.

Whilst these approaches performed considerably better correctly predicting non-mutagenic compounds, the high number of false negatives, 15 and 13 for DEREK and TOPKAT respectively would be a concern if either approach were to be implemented to estimate transformation product toxicity during risk assessment or prioritisation activities. In previous studies it has been suggested that the rate of false negatives could be decreased, generally resulting in an increase in false positives, by combining the estimates from both programs (Cariello et al. 2002). As with other predicted end-points, e.g. physico-chemical properties and ecotoxicity, some of the most accurate estimates for a diverse chemical inventory can be achieved when the predictions from more than one approach are combined (Clarke and Delaney 2003; Clarke et al. 2004; Sinclair and Boxall 2005). However, limited concurrence was observed between DEREK and TOPKAT when positively estimating transformation products that were mutagenic (4 compounds). This lack of concurrence could support the notion that the two approaches are estimating mutagenicity based on different criteria. Predictive ability, particularly through a reduction in false negatives, may be enhanced by:

- adjusting predictive interpretation by considering related endpoints or widening the probability limits (Cariello et al. 2002);
- combining the predictive ability of approaches (Chaudhry et al. 2006); and/or
- considering the experimental or predicted toxicity of the parent pesticides (Sinclair and Boxall 2003; Escher et al. 2006).

Therefore these proposed methods were considered in an attempt to improve identification of mutagenic transformation products. Mutagenicity alerts in DEREK were combined with alerts for carcinogenicity and chromosome damage, within TOPKAT probability limits were relaxed and compounds outside the applicability domain were considered and the mutagenic/genotoxic potential of the parent pesticide, experimental and estimated, were also considered (Table 21; Table 22).

Table 21. The consideration of different predictive interpretation and parent toxicity to predict transformation product mutagenicity and reduce the number of false negatives with DEREK

	parent pesticide is mutagenic/ genotoxic	estimates parent to be mutagenic	mutagenicity alerts	mutagenicity & chromosome damage alerts	mutagenicity & carcinogenicity alerts
False positives	19	13	7	10	31
False negatives	7	13	15	8	12
True positives	11	5	3	9	6

Table 22. The consideration of different predictive interpretation and parent toxicity to predict transformation product mutagenicity and reduce the number of false negatives with TOPKAT

•	Parent pesticide is mutagenic/ genotoxic	estimates parent to be mutagenic [b]	standard[a] ≥ 70% +'ve ≤ 30% -'ve	≥ 60% +'ve ≤ 40% -'ve	ignore OPS
False positives	19	8	12	12	21
False negatives	7	7	13	13	13
True positives	11	3	2	3	3

[a] – two mutagenic transformation products had an indeterminate estimate of mutagenicity
[b] – eight pesticides had estimates outside the applicability domain

Relaxation of the probability limits had not effect on the number of false negatives for TOPKAT whilst ignoring the optimum prediction space increased the number of false positives. Conversely when the applicability domain has been ignored previously this has had little effect on predictive ability (Cariello et al. 2002). The inclusion of alerts for carcinogenicity in DEREK decreased false negatives but considerably increased false positives from 7 to 31 compounds, whilst the inclusion of chromosome damage rather than carcinogenicity reduced false negatives from 15 compounds for mutagenic alerts to only 8 compounds

with only a limited increase in false positives, from 7 to 10 compounds. Only seven compounds, from eighteen, were false negatives for mutagenicity if the transformation product was attributed the experimental mutagenic/genotoxic potential of the parent pesticide. This is logical if the transformation products exhibit only a small change in molecular structure during degradation then they could still maintain the structural moieties responsible for the effect. Therefore if parental experimental mutagenicity was considered together with DEREK alerts of mutagenicity and chromosome damage and TOPKAT using the standard predictive interpretation then this combined approach produced only one false negative, seventeen mutagens correctly identified and 33 false positives from the remaining 105 non-mutagens. Combining predictive approaches in a similar manner to estimate the mutagenic potential has also provided improvement in overall performance for pharmaceuticals (White et al. 2003).

6.3.2.2 Rat oral lethality

TOPKAT could not provide rat oral LD_{50} estimates for four transformation products due to parameterisation problems and thirteen compounds were outside the optimum prediction space and the optimum prediction space limits. Where exact numerical values were available and TOPKAT could provide a valid estimate, 81.8% of estimates where within an order of magnitude of experimental values. The potency of 53% of transformation products was overestimated with four overestimated by more than an order of magnitude; DTPU and TPSA from flazasulfuron, IM-2-1 from acetamiprid and INN-79 from oxamyl. The transformation products that had their potency most underestimated were produced from the degradation of the organophosphorus insecticide diazinon, namely TEPP and O,S-TEPP. For experimental data reported as an inequality, 51% of transformation product estimates were more potent that the reported greater than value. There is therefore a slight tendency for TOPKAT to overestimate the potency of transformation product rat oral LD_{50} values (Figure 21). This could therefore provide the user with a conservative estimate that is more favourable than the reverse when undertaking a prioritisation to evaluate hazard. Rat oral LD_{50} models within TOPKAT were

developed using data from the Registry of Toxic Effects of Chemical Substances (RTECS) and during development if multiple values were identified for a single compound then the most potent was used within the training set of the model (Anon. 2004), thereby providing the model with a tendency to estimate that compounds are more potent than substantiated by some of the experimental data. During a previous evaluation of TOPKAT to estimate this end-point for an extensive chemical dataset, the Danish EPA concluded that performance was poor (r^2 = 0.31), however 86% of results were within an order of magnitude of experimental values, similar to the results here (r^2=0.12, 82%), and it was suggested that the approach is appropriate to give an approximation of toxicity (Danish EPA 2001).

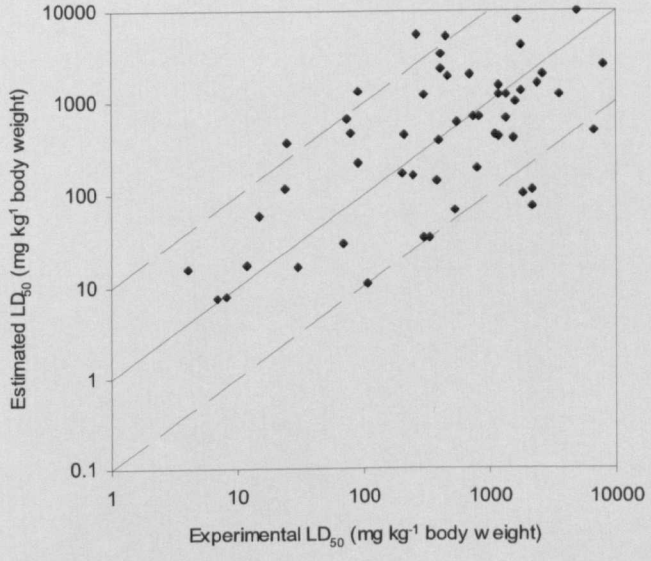

Figure 21. Comparison of experimental rat oral LD_{50} values and those estimated by TOPKAT for transformation products (where experimental values where reported as numerics) (solid line x=y, hashed lines equal one order of magnitude under or over estimated)

6.3.3 The Risk of Transformation Products Formed from High Use Pesticides

In the proposed methodology to rank transformation products on their potential risk to humans through the consumption of drinking water in a catchment, parental pesticide ADI was used for the hazard component as a surrogate for transformation product mammalian toxicity since these data are scarce (Chapter 5). Using ADI could over-estimate (or underestimate) the potency of some transformation products, since this approach assumes transformation product toxicity is equivalent to the parental pesticide toxicity. The potential risk of transformation products formed from the ten most used pesticides in the US (Gianessi and Reigner 2006a; Gianessi and Reigner 2006b) and Great Britain (Thomas Pers. Comm. 2008) were prioritised for their exposure to drinking waters supplies according to the exposure component of the approach proposed in Chapter 5. The potential ranking of these transformation products where hazard was expressed using parental ADI against estimates of transformation products rat oral LD_{50} and mutagenicity as discussed earlier was investigated. To provide a ranking score, a system just incorporating rat LD_{50} and mutagenic potential similar to that proposed by Capelton et al. (2006) was used (Table 23).

29 transformation products were identified from the ten most used pesticides in the US and 23 from the ten most used pesticides in Great Britain, chlormequat, the most used pesticide in Great Britain by weight of active ingredient had no environmental transformation products identified. Environmental formation data as a result of parent pesticide degradation were collated from a range of documents (EPA 2007; PSD 2007; EU 2007b; EU 2007b; PMRA 2007c; EFSA 2007e) as were persistence and mobility. Where absent, mobility data (K_d) were estimated using the approach proposed in Chapter 3, the octanol-water partition coefficient (K_{ow}) was estimated from the average of three approaches; CLogP (BioByte Corporation), ALogPS (Virtual Computational Chemistry Laboratory) and KOWWIN (Syracuse Research Corporation). This is then transformed to organic carbon normalized adsorption coefficient (K_{oc}) using the quantitative

structure property relationship (QSPR) of Kanazawa (1989) and then the distribution coefficient (K_d) is determined assuming a soil organic carbon content of 2% (ECB 2003). Transformation products without experimentally determined persistence data ($DT_{50}/t_{½}$) were allocated the 75th percentile of values from the collated experimental persistence data (30 days) since no adequate predictive approach has been identified (Chapter 3).

Table 23. A system to score pesticide transformation products based on their estimated mutagenicity and rat oral toxicity

End-point	Score [d]	Criteria	
Rat oral LD_{50}	0	<1 mg kg^{-1} body weight	(extremely high toxicity)[a]
	4	1 – 9 mg kg^{-1} body weight	(high toxicity) [a]
	6	10 – 49 mg kg^{-1} body weight	(high toxicity) [a, c]
	7	50 – 99 mg kg^{-1} body weight	(moderate toxicity) [a]
	8	100 – 499 mg kg^{-1} body weight	(moderate toxicity) [a]
	9	500 – 999 mg kg^{-1} body weight	(low toxicity) [a]
	10	1000 – 4999 mg kg^{-1} body weight	(low toxicity) [a]
	11	5000 – 9999 mg kg^{-1} body weight	(very low toxicity) [a]
	12	≥ 10000 mg kg^{-1} body weight	(very low toxicity) [a]
Mutagenicity (genotoxicity)	0	Parent pesticide exhibits mutagenicity or DEREK identifies alerts in the transformation product for mutagenicity or chromosome damage or TOPKAT estimates the transformation product to be a mutagen	
	3	All required data/estimates are not available [b]	
	6	Parent pesticide does not exhibit mutagenicity and DEREK does not identify alerts in the transformation product for mutagenicity or chromosome damage and TOPKAT estimates the transformation product to be a non-mutagen	

[a] – Hodge and Sterner scale 1949
[b] – Either parental pesticide mutagenic/genotoxic potential is not available, DEREK or TOPKAT are unable to process the molecule or the molecule falls outside the applicability domain of TOPKAT
[c] – If valid rat oral LD_{50} estimates were not possible molecules were given a score of 6
[d] – Once attributed the scores were normalised to provide values within an equivalent order of magnitude of ADI values by dividing by 200

Table 24 provides those transformation products with the most potent scoring according to the system in Table 23 and their respective parent pesticide ADI and their exposure index calculated according to the approach in Chapter 5. This example only considers a limited number of transformation products, when compared to the total number that could be expected to be formed following pesticide application within a catchment, however they are all from high use pesticides (>4000 tonne yr^{-1} US and >275 tonne yr^{-1} Great Britain). Including a consideration of transformation product estimated toxicity provides information

on those compounds that may pose a hazard from these high use pesticides. The transformation product of trifluralin, 2-ethyl-7-nitro-1-propyl-5-(trifluoromethyl) benzimidazole is allocated the most potent score (4) since the estimated rat oral LD_{50} is 7.4 mg kg^{-1} body weight, categorised as a high toxicity and both DEREK and TOPKAT estimate that this compound will be mutagenic. In terms of identifying possible substance of concern for further investigation this compound is ranked relatively low for both exposure (26/29 in the US and 20/23 in Great Britain) and toxicity of its parent pesticide (12/29 in the US and 14/23 in Great Britain) highlighting that estimation of mammalian toxicity in the absence of experimental data could be another tool used to narrow the field when considering whether any transformation products pose a risk to consumers via drinking water.

Table 24. Estimated toxicity score of transformation products formed from the ten most used pesticides in the US and Great Britain

Transformation product	Parent pesticide	Transformation product toxicity score [a]		Transformation product exposure index [b]		Parent pesticide ADI (mg kg^{-1} bw d^{-1})	
		value	rank	value	rank	value	rank
US							
2-ethyl-7-nitro-1-propyl-5-(trifluoromethyl) benzimidazole	trifluralin	4	1	1.78E-06	26	0.024	12
2-ethyl-7-nitro-1-propyl-5-(trifluoromethyl) benzimidazole-3-oxide	trifluralin	6	2	1.08E-06	28	0.024	12
methylisothiocyanate	metam sodium	8	3	2.98E-03	8	0.01	9
nitromethane	chloropicrin	8	3	2.04E-03	11	0.001	1
chloronitromethane	chloropicrin	8	3	2.57E-04	15	0.001	1
cis-3-chloroallyl alcohol	1,3-D	8	3	8.63E-05	17	0.025	17
trans-3-chloroallyl alcohol	1,3-D	8	3	5.78E-12	29	0.025	17
2,4-dichlorophenol	2,4-D	9	8	2.36E-04	16	0.05	21
2,4-dichloroanisole	2,4-D	9	8	1.58E-04	19	0.05	21
2-ethyl-7-nitro-5-(trifluoromethyl) benzimidazole	trifluralin	9	8	1.14E-05	24	0.024	12
Great Britain							
2-ethyl-7-nitro-1-propyl-5-(trifluoromethyl) benzimidazole	trifluralin	4	1	6.01E-06	20	0.024	14
2-ethyl-7-nitro-1-propyl-5-(trifluoromethyl) benzimidazole-3-oxide	trifluralin	6	2	3.63E-06	22	0.024	14
3-cyano-2,4,5,6-tetrachlorobenzamide	chlorothalonil	6	2	6.92E-04	2	0.015	6
3-cyano-6-hydroxy-2,4,5-trichlorobenzamide	chlorothalonil	6	2	2.06E-04	9	0.015	6
4-hydroxy-2,5,6-trichloroisophthalonitrile	chlorothalonil	6	2	1.07E-05	18	0.015	6
3-cyano-2,5,6-trichlorobenzamide	chlorothalonil	8	6	3.71E-04	6	0.015	6
acetaldehyde	metaldehyde	8	6	3.41E-04	8	0.025	19
ethylenethiourea	mancozeb	8	6	4.01E-226	23	0.03	21
2-ethyl-7-nitro-5-(trifluoromethyl) benzimidazole	trifluralin	9	9	3.83E-05	14	0.024	14
paraldehyde	metaldehyde	9	9	1.61E-05	16	0.025	19

[a] – Toxicity score according to estimated rat oral LD_{50} and mutagenic potential following the scoring provided in Table 23

[b] – Transformation product exposure index calculated according to Sinclair et al. (2006)

In the UK the regular monitoring of pesticide transformation products in both surface and groundwaters and raw and finished drinking waters by the Environment Agency and water companies, respectively, is generally limited to the determination of transformation products of the organochlorine insecticides DDT and heptachlor, active ingredients which have not been used in the UK for a number of years. Over the past 5 years very limited monitoring has been carried out for any other transformation products and following current regulations there are no requirements to measure the levels of transformation products other than those mentioned in Guidance (DWI 2008). Whilst in the US, transformation products, particularly from herbicides are routinely monitored for by the USGS.

Transformation products from intensively used herbicides have been identified in finished drinking waters ready for distribution (Coupe and Blomquist 2004; Hladik et al. 2006). Whilst some drinking water treatment methods, such as activated carbon adsorption, reverse osmosis and nanofiltration can remove pesticides and their transformation products associated with the aqueous phase (Wang and Song 2004), there is the potential for harsh disinfection processes such as oxidation using ozone, hydrogen peroxide or UV radiation to transform organic compounds present in the raw water to alternative compounds (Nguyen et al. 2004). Recently, concern over the potential toxicology of compounds formed from environmental transformation products of certain pesticides following drinking water treatment led to their (temporary) commercial withdrawal (European Commission 2007).

Predictive techniques are available that can be used to estimate the biodegradation of chemicals (e.g. Jaworska et al. 2002), however when these are examined for their ability to correctly identify environmental pesticide transformation products their performance for a range of pesticides is very variable. The identity of transformation products formed in soil from some pesticides can be predicted whilst others have none correctly identified (Sinclair et al. 2003). No predictive approaches are currently available to identify the

structure of compounds that maybe formed from pesticides and their environmental transformation products during drinking water treatments, but approaches are available to determine how reactive organic contaminats are to harsh treatments such as chlorination or ozonation (Lei and Snyder 2007). Such techniques can help indicate the most reactive and therefore the most likely to form treatment by-products which in the absence of predictive tools can focus the efforts of experimental studies investigating by-product identity. When such research is further developed, we can begin to assess the hazard posed by by-products produced during drinking water treatment using mammalian estimation approaches such as DEREK and TOPKAT, to get a measure of whether they pose a risk to consumers.

The predictive power of estimation techniques is based on the experimentally determined toxicological knowledge of compounds present in their training set, and whilst interpolation between similar chemicals, within limits, for the same toxicological response can be undertaken these approaches are unable to estimate new effects not previously identified. For this reason, it is unlikely that predictive techniques will completely replace experimental determination of some of the most important end-points, particularly for biologically active molecules such as pesticides and pharmaceuticals. However these techniques have an important role in aiding the implementation of the 3R's and during prioritisation and scoring exercises. Therefore whilst the transformation products under investigation in this chapter can be ranked on their toxicological profile using current knowledge it would be impossible to conclude that certain compounds posed little risk when their effect could be via a yet unidentified mode of action.

6.4 Conclusions

Generally pesticides demonstrate a greater mammalian toxicity than their transformation products, however some compounds can exhibit an increased toxicity or exhibit toxicity not seen in the parent pesticide. When the predictive

ability of TOPKAT and DEREK are compared to experimentally determined data, they perform better when estimating compounds that are non-toxic than attributing a toxicity to a transformation product, however the number of false negatives can be decreased when these approaches are used together and the toxicity exhibited by the parent pesticide is also considered. Parental pesticide ADI may not be a suitable surrogate for transformation product toxicity and predictive approaches maybe a more suitable approach for providing information on their toxicity in the absence of experimental data. Moreover with the implementation of the 3R's and in the face of the large number of transformation products formed in the environment and the number of additional compounds that maybe created during drinking water treatment, predictive techniques will play a role in prioritisation and ranking exercises to identify those that maybe of concern.

7 Final Discussion and Conclusions

7.1 Introduction

During risk assessment activities transformation products do not receive the attention of their pesticidal parents. Generally, due to constraints of time and money experimental testing is limited to one major transformation product with little or no consideration given to the remainder of the compounds produced during pesticide degradation. Therefore this thesis has developed and explored approaches for determining through non-experimental means the fate, occurrence, ecotoxicity and toxicity of pesticide transformation products. This thesis was written over a seven year period and many of the chapters are based on scientific papers published at the time of writing. During this time the field of transformation product risk assessment, particularly the estimation of ecotoxicity, has been moving rapidly, so in this final chapter:

1, The proposed approach to assess aquatic ecotoxicity is evaluated against a newly available dataset and comparisons are made with approaches now available from other research groups;
2, Two case studies are used to illustrate how the methodologies proposed and evaluated throughout this thesis can be applied to the environmental assessment of transformation products; and
3, Finally, major knowledge gaps are identified, overall conclusions from this research are presented and recommendations made on future research priorities in the area of transfromation product risk assessment.

7.2 Evaluation of approach(es) to estimate aquatic ecotoxicity

On the basis of the investigation of available acute aquatic data and development of the reasoning, a pragmatic approach was developed in Chapter 4 to allow the user to generate a conservative estimate of transformation product aquatic

ecotoxicity to non-target organisms (fish, daphnids and/or green algae) in the absence of experimental data. This approach uses information on parent pesticide ecotoxicity and properties and the properties and structure of the transformation product. During its development the approach was not evaluated against data not used in its development or tested against the performance of other methodologies. This was due to; 1) the lack of additional ecotoxicological data against which to evaluate the approach because all the limited available data was required to generate a suitable training set, and 2) no other pesticide transformation product specific estimation methodologies were available against which to test the proposed approach. This however is not the current situation, additional data on acute daphnid ecotoxicity of 92 transformation products were collated from newly available regulatory review documents (EFSA 2009, EPA 2009, PMRA 2009, PSD 2009b) and used to test the proposed approach and compare its performance to approaches developed for transformation products; 1) DEMETRA (Benfenati 2007) and 2) the approach of Escher et al. (2006). To also ascertain whether approaches developed specifically for pesticide and/or pesticide transformation products are required or whether approaches developed using chemicals from other chemical classes can be used, the commonly utilised QSAR approaches ECOSAR (EPA) and TOPKAT (Accelrys Inc.) were also included in the evaluation.

The approach proposed in Chapter 4 was developed with a combination of ecotoxicity data from three trophic levels since data availability for individual trophic levels was insufficient. Fifty-seven daphnid data points were used during development, therefore it can be considered that the use of 92 data points to test the approach is rather disproportionate. Generally when predictive techniques are developed, collated data is randomly divided into a training set and a test set, generally in a 70% to 30% ratio, respectively. Based on the evaluation with new daphnid ecotoxicity data it appears that the approach does not provide a conservative estimate for all of the transformation products within the test set (Figure 22). Fifty-one transformation products had their daphnid ecotoxicological potency conservatively estimated, whilst the potency of twenty-

nine was underestimated, with five more than two orders of magnitude underestimated, i.e. not providing the anticipated or desired conservatism for risk assessment and/or prioritisation exercises.

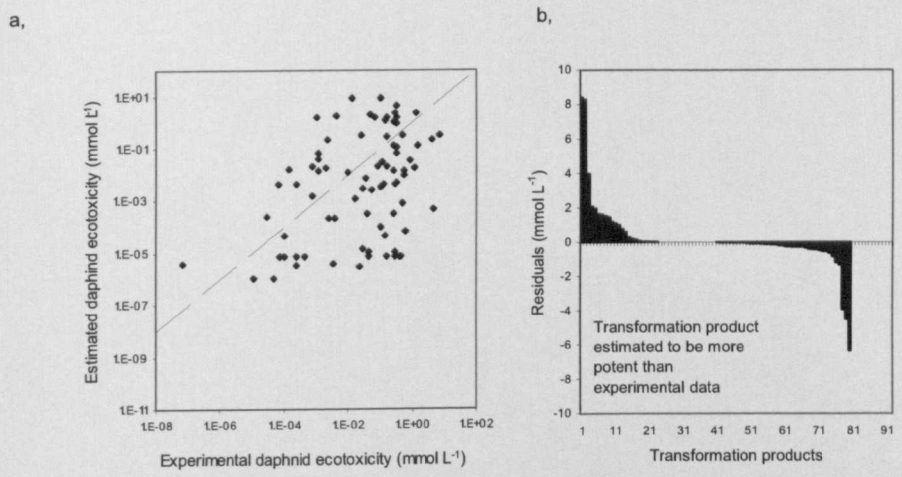

Figure 22. Performance of the approach proposed in Chapter 4 at estimating daphnid acute ecotoxicity (48h EC_{50}) for a dataset of 92 transformation products; a, correlation with experimental data (dashed line x=y) and b, residual plot (positive = underestimation)

During the determination of assessment factors (Chapter 4, Figure 4), the daphnid data utilised does not appear to have been totally representative for all transformation product potency to daphnids. When the data used for this evaluation is plotted in the same manner as the data used to develop the assessment factors it is clear that the determined assessment factor values are not always appropriate (Figure 23). With the significant increase in the availability of transformation product ecotoxicological data for daphnids and other aquatic taxa such as green algae, fish as well as *Lemna sp.*, then it appears the assessment factors need to be re-evaluated, maybe producing taxa specific assessment factors rather than the taxa generic values determined during Chapter 4. Examining the data in Figure 23 it appears that an assessment factor of 0.01 for transformation products that contain the parental pesticide toxicophore and an assessment factor of 0.1 for the remaining transformation products could be appropriate daphnid specific assessment factors, moreover the application of a

safety factor, e.g. 0.1, may be prudent to ensure the conservative nature of the approach.

a,

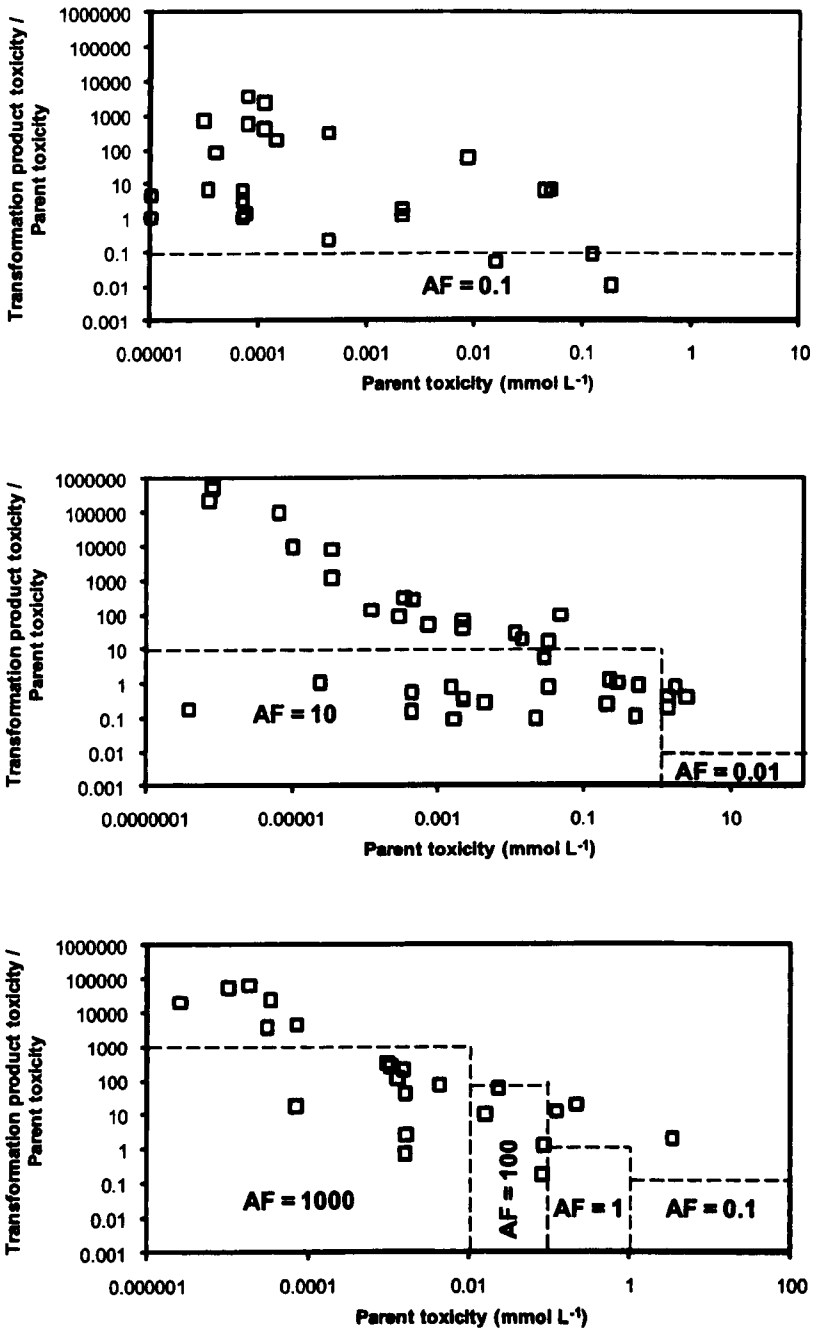

Figure 23. Evaluation of approach proposed in Chapter 4 using daphnid ecotoxicity data for 92 transformation products (dashed lines represent the taxa generic assessment factors)

7.2.1 Comparisons with newly available approaches

At the time the approach proposed in Chapter 4 was developed no other tools were available specifically to estimate acute aquatic ecotoxicological endpoints for pesticide transformation products, i.e. fish 96h LC_{50}, daphnid 48h EC_{50} and green algal 72h EC_{50}. Alternative approaches have subsequently been developed for generating ecotoxicity estimates for these compounds, some as a result of the publishing of the proposed approach. The DEMETRA QSAR program, freely available on the internet, was the result of a large EU project with numerous international collaborators. This approach is reported to be suitable to estimate the aquatic ecotoxicological (fish and daphnid) and terrestrial ecotoxicity (bird and bee) for pesticides and transformation products, even though no ecotoxicity data for transformation products were used during its development (Benfenati 2007). In addition an expert system based on the principal of the toxic ratio (Verhaar et al. 1992) has been proposed by Escher et al. (2006) which can provide the potential ecotoxicological range of a transformation product on the basis of the potency of the parent compound and the use of narcotic QSARs. This approach was originally developed using transformation products of human pharmaceuticals but is equally applicable to transformation products of pesticides (Escher et al. 2009).

The approach proposed by Escher et al. (2006) provides a methodology for estimating the ecotoxic range of a transformation product, for the purposes of this evaluation the most potent extreme of that range was used as the prediction against which experimental data were compared. This approach uses the principle of the toxic ratio proposed by Verhaar et al. (1992) which is the ratio between baseline (or narcotic) toxicity and the toxicity determined experimentally for the end-point under investigation. Applying this approach involves calculating the toxic ratio of the parent pesticide using available experimental data and by estimating baseline toxicity using a recommended non-polar narcotic QSAR (ECB 2003). The maximum potency of the transformation

product can then estimated by applying the toxic ratio of the parent pesticide to the baseline toxicity estimate of the transformation product.

DEMETRA is a collection of QSAR developed using a wide range of pesticide experimental ecotoxicity data which allows the prediction of pesticide (and transformation product) ecotoxicity to fish, daphnia, bee and quail (oral and dietary exposure). DEMETRA contains a hybrid combinative model for each endpoint which incorporates intelligent integration of several individual validated QSARs. Transformation product molecular descriptors are generated from structural files (.mol) using Dragon (Milano Chemometrics) and entered into DEMETRA to generate the estimates for daphnid ecotoxicity.

ECOSAR is a freely available software system which matches the structure of a query molecule to one (or more) of its defined chemical class(es). For most classes, aquatic ecotoxicity values are predicted using available linear correlations between toxicity and hydrophobicity, if not available experimentally K_{ow} is estimated for the query molecule using KOWWIN. For the purposes of assessing transformation product daphnid ecotoxicity in instances where the query compound was matched to one or more chemical classes, the most potent ecotoxicity estimate for daphnids was selected for comparative purposes.

TOPKAT is a commercially available system and contains a range of cross-validated QSARs, which are multivariate statistical relationships between experimentally derived toxicity data and chemical descriptors that quantify chemical transport properties and biochemical interaction with the target site. It also provides the user with a measure of whether the query molecule fits within the prediction space of the chosen relationship and therefore whether the estimation is reliable. For this comparison exercise, estimated daphnid data were only compared if they fell within the optimum prediction space or outside but within a permissible range as determined by TOPKAT.

To measure predictive performance the statistics developed in Chapter 3 were used (number of chemicals from the test set an estimate could be generated, percentage positive deviation, mean absolute deviation, mean squared absolute deviation, percentage of compounds greater than an order of magnitude greater than experimental values and the Pearson correlation coefficient).

When quantifying the accuracy with which the approach proposed in Chapter 4 can estimate daphnid ecotoxicity with the ability of other available methodologies, a poor performance was initially anticipated since the proposed approach was developed to provide a conservative estimate, i.e. a value more potent than experimental data would suggest, whilst the other methods against which it was to be compared were designed to accurately estimate experimental values (apart from that of Escher et al.). However in the previous section it was demonstrated that the proposed approach is not as conservative as first anticipated. The performance of the four comparative approaches can be seen in Figure 24.

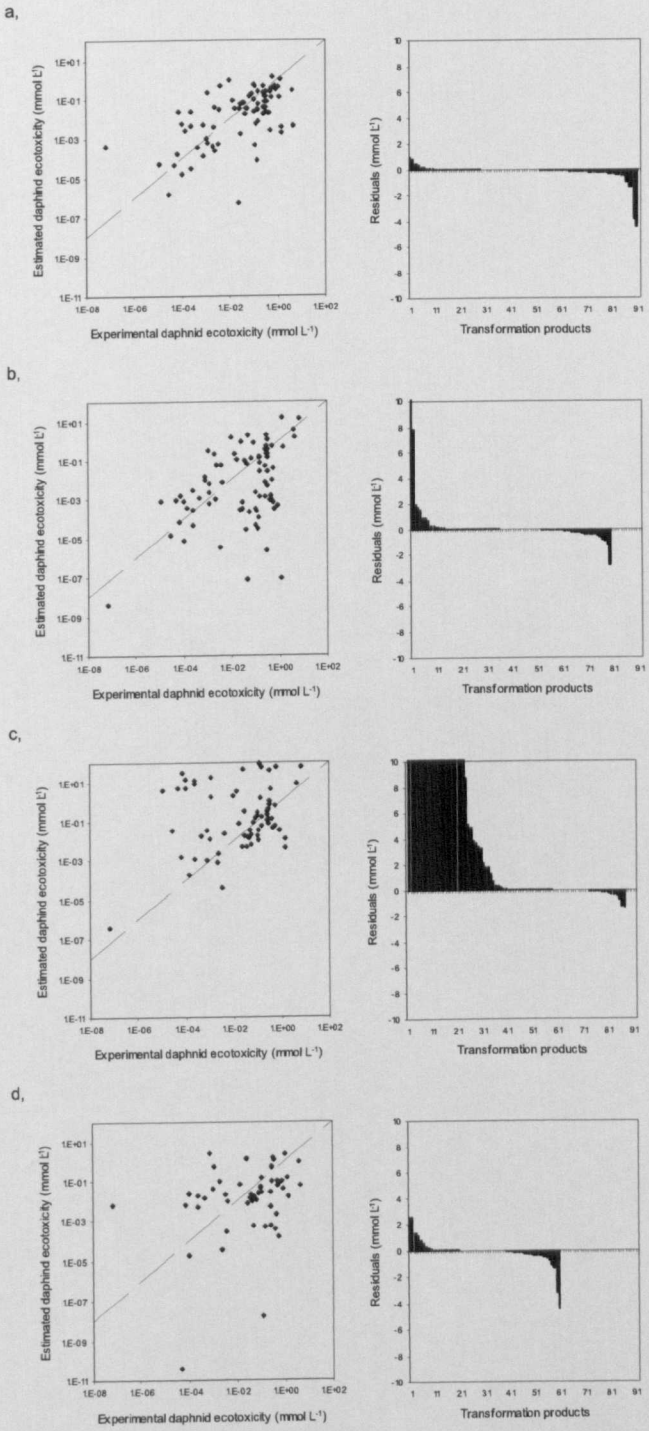

Figure 24. Correlation with experimental daphnid ecotoxicity data (dashed line x=y) and residual plot (positive = underestimation) for a, DEMETRA, b, Escher et al., c, ECOSAR and d, TOPKAT

TOPKAT performed well but was limited by the number of compounds it could provide a valid estimate (66%) and ECOSAR had a significant tendency to underestimate toxicity with 59 compounds underestimated, 28 by two orders of magnitude or more. Both 'general' approaches were out-performed by those developed specifically for the estimation of pesticide and/or transformation product ecotoxicity, which indicates that approaches used to estimate transformation product ecotoxicity should be based on pesticide and/or transformation data rather than data for general chemicals. The approach proposed in Chapter 4 performed better than the general approaches but was out performed by DEMETRA and the approach of Escher et al. (Table 25). Based on the statistics the approach of Escher et al. was the best performer overall and was not the poorest performer in any of the selected statistical parameters. This is surprising as this approach is based on a relatively simple concept and indicates that transformation product toxicity is substantially linked to that of its parent pesticide, or at least for transformation products within this evaluation dataset.

Table 25. Rank scores for the statistics selected with which to evaluate the performance of five approaches for estimating transformation product ecotoxicity to daphnids (48h EC50)

Statistics	Rank scores for				
	Proposed approach	DEMETRA	Escher et al	ECOSAR	TOPKAT
Number of chemicals	0.387	0.032	0.387	0.129	1
Percentage positive deviation	0.758	1	0.276	0.940	0.859
Mean absolute deviation	0.008	0.003	0.006	1	0.005
Mean squared absolute deviation	<0.001	<0.001	<0.001	1	<0.001
% of compounds > 1[a]	1	0.417	0.763	0.709	0.645
Pearson correlation coefficient	1	0.796	0.343	0.542	0.833
Overall mean rank score	0.53	0.37	0.30	0.72	0.56

[a] – order of magnitude greater than experimental values

7.2.2 Combining approaches for aquatic ecotoxicity estimation

When the individual approaches were evaluated, it was apparent that some approaches performed better than others with the majority of techniques

considerably over or under estimating the potency of some compounds. Generally these compounds, commonly known as 'outliers', fall outside the predictive space of the technique in question producing an inaccurate estimate of ecotoxicity. Therefore to increase the accuracy of transformation product ecotoxicity estimation it would seem prudent to develop a structured methodology that allows the selection of the most accurate/appropriate method. The simplest way of combining approaches would be to generate a conservative estimate of transformation product ecotoxicity, i.e. estimating ecotoxicity using all approaches and then selecting the most potent prediction (Figure 25a). Combining approaches in this manner would provide a conservative estimation of ecotoxicity that could be used in a low tier of the risk assessment process, and if no appreciable risk is identified with the conservative estimate then it would be a waste of resources developing a more accurate estimate and/or an experimentally derived value as this will in all likelihood just reduce the already low risk, which has been identified as acceptable.

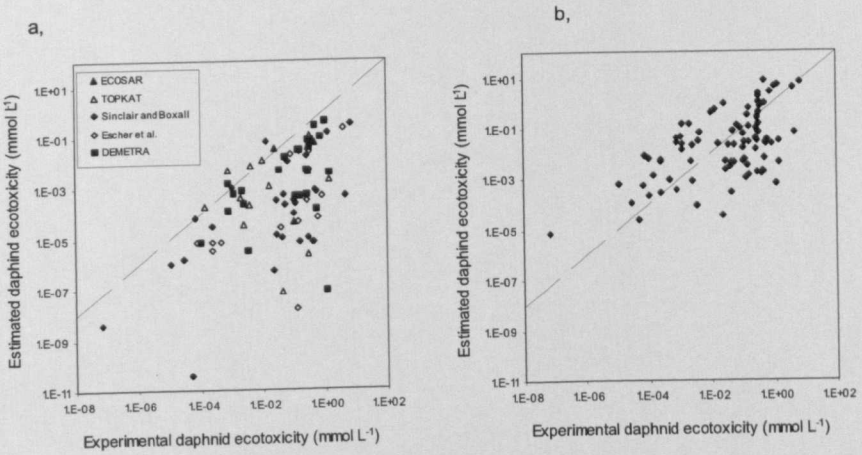

Figure 25. A comparison of daphnid acute ecotoxicity data for 92 transformation products a, the most potent estimates and b, the geometric means provided by the five evaluated approaches (dashed line x=y)

Combining techniques with a structured methodology would allow the selection of the most accurate/appropriate method and would reduce the impact of outliers when compared to using an individual technique. Techniques could be

combined and hence increase predictive ability by using an average of these estimates as previously suggested for the prediction of physico-chemical properties (Clarke et al. 2004). When generating an average the geometric mean is the most appropriate as this would reduce the impact of significant outliers (e.g. Figure 25b). However it would be more prudent to develop a rule-based methodology that allows the user to select the most appropriate/accurate technique for the specific query transformation product. This would require a thorough investigation into: 1) quantifying the predictive domain of each suitable approach, 2) rationalising the identity of outliers for each approach and 3) identifying which chemical types/categories are most appropriate for each approach. Developing such an approach would require a large transformation product dataset that extensively covers a range of taxa, physico-chemical properties, transformation product chemical classes and parent pesticidal chemical classes.

7.3 Environmental assessment of transformation products

It is important that transformation products are included during any risk assessment activities for pesticides as they can add significantly to the overall impact (Kolpin et al. 2001; Gasser et al. 2007). The aim of this thesis was to investigate and develop pragmatic approaches for assessing the fate and effects of transformation products in the absence of experimentally determined data. Throughout this work various approaches have been proposed and/or evaluated. Such approaches maybe used by organisations requiring knowledge on pesticide transformation products but their reasons maybe quite different. Some may need to determine the specific risk of individual transformation products whilst others may need to identify those compounds from a plethora that need further consideration. The approach taken will be dependent on the scope and requirements of the results, some organisations maybe considering the downstream implications of pesticide usage and transformation product formation in waters and may want to identify those compounds that are of most

concern, e.g. drinking water companies, beverage and food manufactures or regulators of these commodities. Whilst other organisations may want to identify the exposure or hazard from transformation products formed from a specific pesticide in the absence of experimental data e.g. agrochemical companies or pesticide regulators. Therefore two case studies with worked examples are described in the subsequent sections through which the appropriate organisations can work to provide their required data and outcome.

7.3.1 Potential contamination of source waters

The contamination of water by pesticides and some transformation products abstracted for human consumption has been well documented (e.g. Hladik et al. 2006) and is why many water treatment plants employ sorption technologies to remove these organic contaminants, e.g. activated carbon. Water can be the integral component of some companies' final products, e.g. canned beverages, and like all their ingredients foremost producers generally want to ensure that their raw ingredients are of the highest quality. If contamination of their finished product is identified it may severely impact their sales and/or reputation. Therefore analytical screens are routinely employed and generally contain ranges of target pesticides but generally no transformation products. The range of contaminants can be so vast e.g. when considering pesticide transformation products, companies may want to undertake a prioritisation, as suggested in Chapter 5, to identify the most probable potential contaminants. Required data can either be collated from the literature or from the review and detailed data tables presented in Chapter 2 and Appendix A. In the absence of experimental data information on physico-chemical properties and mammalian toxicity can be estimated by the methods described in Chapter 3 and Chapter 6 respectively. Figure 26 presents a flow diagram detailing a methodology of how those transformation products that may need adding to an analytical screen can be identified.

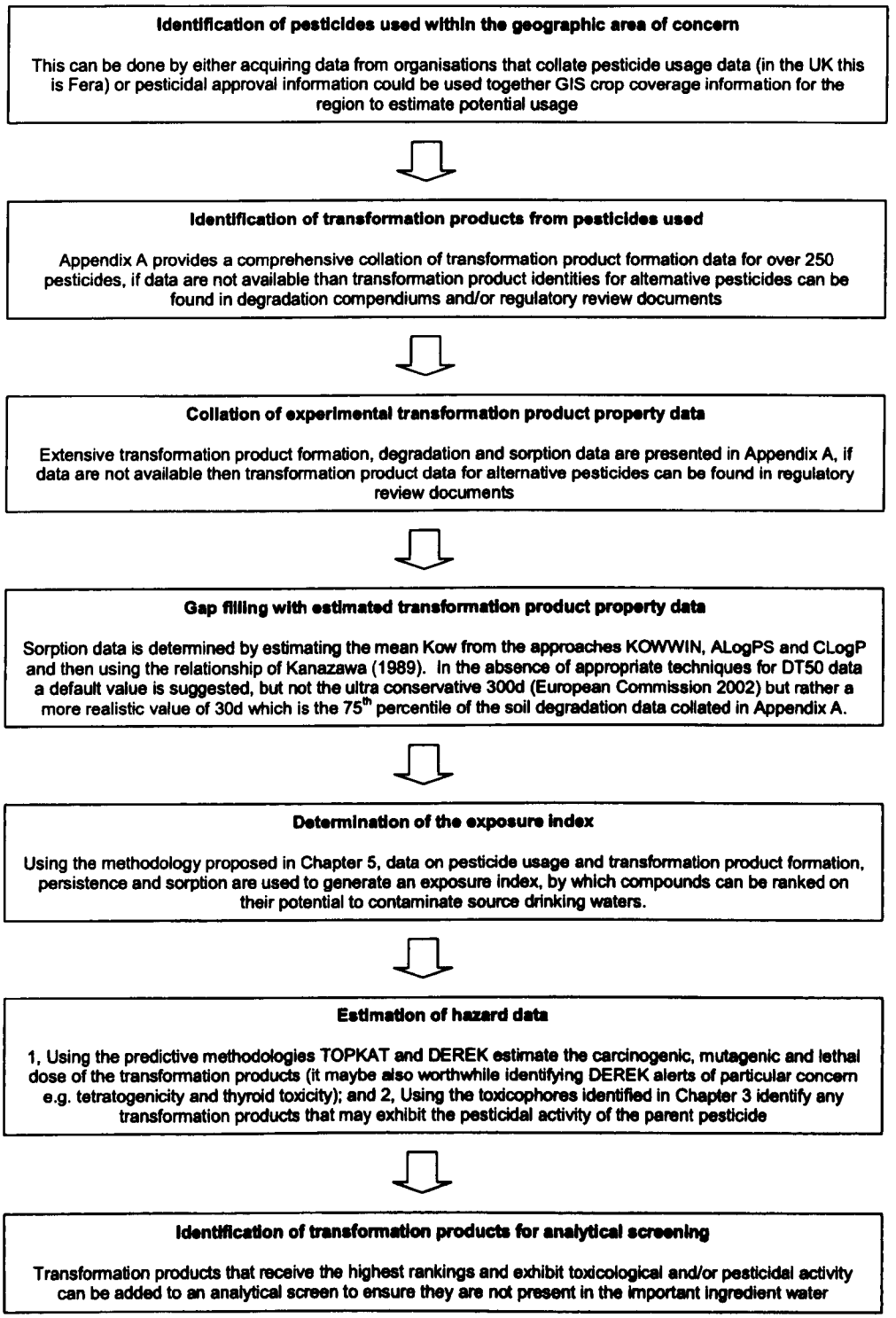

Figure 26. Proposed approach for beverage manufacturers to identify which transformation products they should add to their regular analytical screens

7.3.1.1 Transformation product analytical determinand list

This example considers a fictitious company based in York, North Yorkshire that uses large volumes of locally sourced water in the production of their canned beverage products. To ensure quality and safety the company wish to add the most important pesticide transformation products to their routine source water analytical screen. Below is a summary of the stages to be performed following the protocol proposed in Figure 26 to identify the compounds to be added to the analytical screen.

- Pesticide usage data for North Yorkshire was obtained from the Pesticide Usage Survey Team at the Food and Environment Research Agency. These data comprised the identity of 209 pesticides used in the area, together with estimates of their usage per annum.
- Using Appendix A together with regulatory review documents and pesticide degradation compendiums 410 transformation products formed from the pesticide were identified.
- Experimental formation data (all compounds), sorption data (89 transformation products), soil persistence data (56 transformation products) and water persistence data (24 transformation products) were collated from Appendix A.
- In the absence of experimental data, sorption data were estimated for 286 compounds by first generating a combined estimate of K_{ow} using KOWWIN, CLogP and ALogPS and then using this as the input parameter in the relationship of Kanazawa (1989). Thirty transformation products were given a default value for K_d of 0.2 since estimation was not possible due to a lack of structural data. Compounds without soil persistence data were given a default DT_{50}/t½ values of 30d.
- The exposure index was then calculated for all 405 transformation products and the compounds ranked on this basis. The top 25 had their toxicological hazard estimated using DEREK and TOPKAT and scored according to Table 23 in Chapter 6, the results are provided in Table 26.

- Based on this case study the company should therefore consider including transformation products from 1,3-dichloropropene, chlorothalonil, kresoxim-methyl, chloridazon, isoproturon, cymoxanil and aldicarb in their analytical screen of source water(s).

Table 26. Transformation product risk index for North Yorkshire (compounds ranked on their risk index from high to low)

Pesticide	Transformation product [a]	Exposure Index	Hazard score	Risk index
1,3-dichloropropene	**(EZ)-3-chloroacrylic acid**	0.0124	10	0.2483
chlorothalonil	**R417888**	0.0099	8	0.2483
1,3-dichloropropene	**(EZ)-3-chloroallyl alcohol**	0.0018	8	0.0450
chlorothalonil	**3-carbamyl-2,4,5-trichlorobenzoic acid**	0.0017	11	0.0312
kresoxim-methyl	**kresoxim-methyl acid**	0.0022	16	0.0280
chloridazon	**5-amino-4-chloro-3-(2H)-pyridazinone**	0.0010	8	0.0242
isoproturon	**desmethylisoptoturon**	0.0015	15	0.0202
cymoxanil	**JX915**	0.0011	12	0.0182
cymoxanil	**W3595**	0.0008	9	0.0182
cymoxanil	**KP533**	0.0014	15	0.0181
aldicarb	**aldicarb sulfoxide**	0.0007	10	0.0137
aldicarb	**aldicarb sulfone**	0.0008	13	0.0125
chlorothalonil	**3-cyano-2,4,5,6-tetrachlorobenzamide**	0.0003	6	0.0113
isoproturon	3-[4-(2'-hydroxy-2'-propyl)-phenyl]-methyl urea	0.0004	15	0.0054
cymoxanil	R3273	0.0003	13	0.0052
thiophanate-methyl	carbendazim	0.0003	10	0.0052
chlorothalonil	3-carbamyl-1,2,4,5-tetrachlorobezoic acid	0.0002	11	0.0039
phenmedipham	MHPC	0.0003	18	0.0038
propyzamide	N-(1,1-dimethylacetonyl)-3,5-dichlorobenzamide	0.0003	14	0.0036
propachlor	propachlor oxanilic acid	0.0002	10	0.0034
chlorotoluron	3-(3-chloro-p-tolyl)-1-methylurea	0.0002	13	0.0031
simazine	deisopropylatrazine	0.0002	16	0.0030
chlorothalonil	3-cyano-2,5,6-trichlorobenzamide	0.0002	14	0.0026
atrazine	deethylatrazine	0.0001	16	0.0016
amidosulfuron	HOE 101630	0.0001	18	0.0015

[a] – transformation products suggested to be included on analytical determinand list are in bold

7.3.2 Generation of aquatic ecotoxicological estimates

Since it is stipulated in guidance that alternative techniques can be used to provide aquatic ecotoxicological data for transformation products (European Commission 2002a) then it would be prudent for agrochemical companies to investigate these approaches for meeting their regulatory requirements. Undertaking experimental ecotoxicological studies for the three main taxa can cost tens of thousands of pounds, the use of predictive tools would be considerable less costly and could provide data very rapidly. An approach is proposed in Chapter 4 and in this chapter four additional approaches are

evaluated for their ability to estimate aquatic ecotoxicological end-points for pesticide transformation products. During Chapter 3 tools were evaluated that provide some of the required physico-chemical property data to perform the estimations, assuming that limited data, apart from structure, is known about the query transformation product. Figure 27 presents a methodology that could be employed by an agrochemical company or other stakeholder to generate aquatic ecotoxicological estimates for pesticide transformation products.

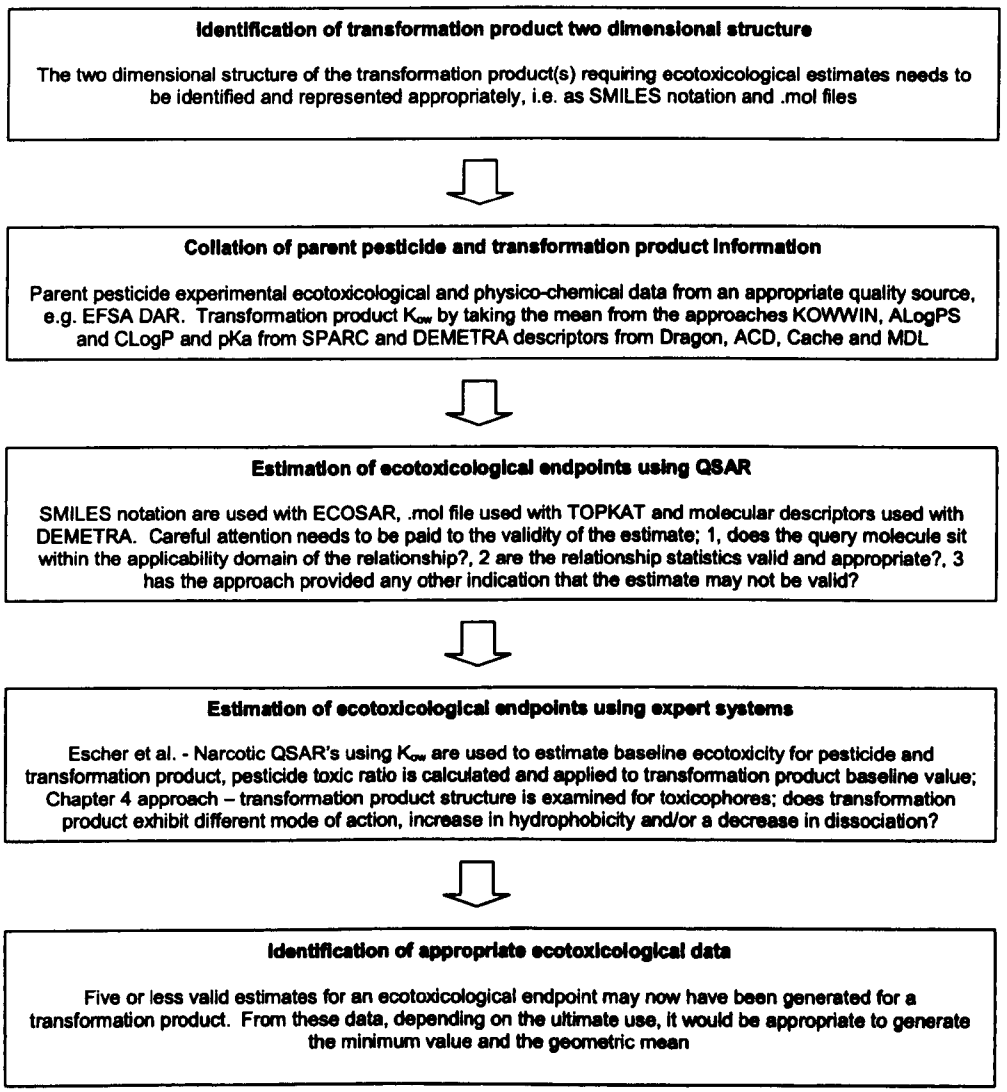

Figure 27. Proposed approach for agrochemical companies to generate ecotoxicological estimates for transformation products

7.3.2.1 Transformation product risk to aquatic organisms

The major thrust of this work has been to evaluate existing and develop new methods to determine the exposure and/or hazard of pesticide transformation products to human health or ecosystems, in the absence of suitable experimentally determined data. This work has evaluated and proposed methodologies for estimating ecotoxicity of transformation products but to determine the risk these compounds pose, these data need to be associated with measures of exposure. Determining the risk of transformation products would: 1) identify whether the risk they pose should be of concern; and 2) identify whether that risk is a significant part of the overall risk posed by the parent pesticide.

In reality non-target aquatic organisms will not be exposed to individual compounds but rather mixtures of the parent compound and some of its transformation products. Moreover, it is probable that aquatic ecosystems that receive water from agricultural land will be exposed to a mixture of different parent pesticides and their associated transformation products in varying concentrations, therefore it can be important to consider the impact of the overall mixture. The mixture risk quotient is a measure that assumes dose additivity assuming that parent pesticides and their transformation products act in the same manner, and can therefore be used as a measure of the risk of a parent pesticide and its transformation products and/or a number of pesticides and their transformation products (Fenner et al. 2002; Boxall et al. 2004). This measure has demonstrated that when a parent compound is solely considered the risk can be acceptable but when the risk from any transformation products are included the overall risk quotient can be greater than one (Fenner et al. 2002).

To consider the risk of transformation products to aquatic ecosystems a unique dataset of parent pesticide and associated transformation products concentrations, monitored in raw surface water abstracted for drinking water were used (Hladik et al. 2006). Risk quotients (mixture and individual pesticide) for five herbicides (alachlor, metolachlor, acetochlor, dimethanamid and

atrazine) and their 28 transformation products were calculated. Individual pesticide and mixture exposure concentrations for peak concentrations identified in the study from six sampling sites in the US, were compared to acute ecotoxicity data for daphnids. In the absence of experimental data ecotoxicity estimates were generated following the approach proposed in Figure 27, ultimately data from the approach of Escher et al. (2006) was used since this was evaluated as the best performing individual technique (Table 25). A summary of the stages performed is provided below.

- Two-dimensional structures for pesticides and their 28 transformation products were collated from regulatory review documents and pesticide degradation compendiums.
- Experimental daphnid ecotoxicity and hydrophobicity data were collated for all pesticides from regulatory review documents. Daphnid ecotoxicity data were also available for two transformation products of alachlor.
- Hydrophobicity (K_{ow}) was estimated for all transformation products using a mean value from KOWWIN, CLogP and ALogPS.
- Daphnid baseline acute ecotoxicity was estimated using the predicted K_{ow} values and recommended narcotic QSAR (ECB 2003). The toxic ratio was estimated for pesticides and then applied to the narcotic estimation of the transformation products to generate a maximum ecotoxicity estimate as proposed by the method of Escher et al. (2006).
- Predicted no-effect concentrations (PNEC) were then generated using the estimated ecotoxicity data and an assessment factor of 100.
- Risk characterisation ratios were then calculated by comparing the measured surface water concentrations against the calculated PNECs.

Overall the risks posed to daphnids from the peak measured concentrations are low (Figure 28), these measured concentrations were for abstracted water, taken from larger water bodies were pesticide and transformation product

concentration will be effected by dilution. The risk posed by metolachlor, acetochlor, dimethenamid and atrazine are all greater than the combined risk of their transformation products, whilst combined the transformation products of alachlor pose a greater (but still very low) risk to daphnids than alachlor itself. This suggests that whilst the risks are low it can be important to include the hazards posed by transformation products as well as the parent pesticide. The only suitable available data to perform such a comparison was for herbicides, insecticides and their transformation products may pose a greater hazard to daphnids but in contrast would probably be present in surface waters at lower concentrations, therefore it is difficult to predict whether combined with their transformation products would pose more or less of a risk to aquatic organisms.

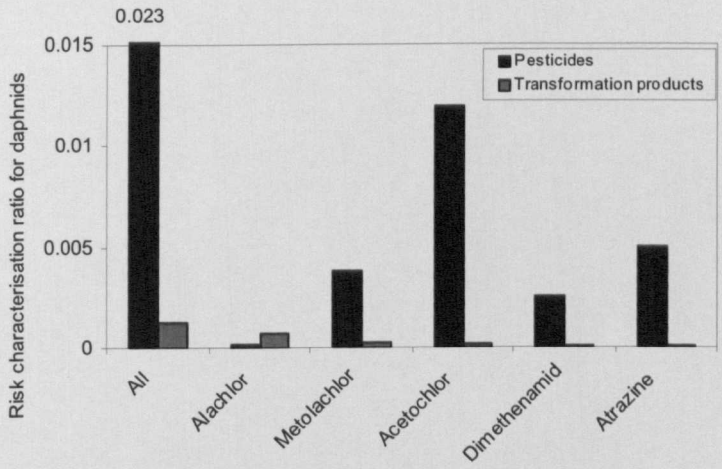

Figure 28. Risk characterisation ratio's for daphnids calculated for pesticides and their metabolites measured in US surface waters

7.4 Major knowledge gaps, overall conclusions and recommendations

Impacts on the environment associated with pesticide transformation products were identified in the late 1960's (Blus et al. 1971) but it is only over the past decade or so that increased attention has been paid to the additional risks posed

by these compounds. In this final section some of the existing knowledge gaps for assessing the risks of pesticide transformation products are discussed, the overall conclusions of the work in this thesis are presented and recommendations made on future work priorities in this area.

7.4.1 Major knowledge gaps

7.4.1.1 Transformation product ecotoxicity

Ecotoxicological hazard, be it aquatic or terrestrial, is a critical parameter to determine for any compound entering the environment with the potential to impact non-target organisms and ecosystems. Compounds such as pharmaceuticals, industrial chemicals and those compounds present in products used in the household can enter environmental compartments following their disposal rather through their intended use. Pesticides are intentionally released into the environment and can subsequently move from site of application, degrade to form transformation products and/or mineralise. It is important that following their application their impact to non-target organisms is limited and that during their evaluation any potential effects caused by their transformation products are considered (Kolpin et al. 2001; Gasser et al. 2007).

Within the EU changes are imminent to the process by which the impact of pesticides are deemed acceptable and therefore gain approval for use (PSD 2009a). The current Directive (91/414/EEC) stipulates that a risk based process (incorporating elements of exposure and hazard) are used to determine whether a pesticide can be placed on the market. It has been suggested that the replacement for this directive will focus more on a hazard based approach. However the details of the new Directive are not clear and under the current Directive and guidance it is detailed that data on transformation product aquatic ecotoxicity does not necessarily need to be addressed with experimental studies but rather alternative methods can be used to generate the required data (European Commission 2002a). At the time this guidance was issued, limited approaches were available to take advantage of the this option for data

generation at a reduced cost, therefore the work performed in Chapter 4 on transformation product ecotoxicity was undertaken. Data were collated and reasoning exploring why some transformation products may exhibit an increased ecotoxicity to non-target aquatic organisms compared to parent pesticides was developed. The majority of occurrences were transformation products were more potent than pesticides could be explained by one of five reasons:

- the applied pesticide acted as a pro-pesticide where the primary transformation product was the active molecule;
- following degradation the parental toxicophore was maintained in the structure of the transformation product;
- the structural change generated a completely different active moiety than that present in the pesticide;
- the transformation product would exhibit increased accumulation due to an increase in hydrophobicity; and
- the transformation product would exhibit increased accumulation due to a decrease in dissociation.

Available acute aquatic data were used to develop this reasoning and it may only be applicable to short-term effects experienced by organisms present in aquatic systems and may not be applicable to explain occasions were transformation products display increased chronic effects. Whilst this is possibly an unusually phenomenon, it is not without precedent since some of the first identified impacts of pesticide transformation products were chronic e.g. egg shell thinning by a transformation product of DDT (Blus et al. 1971). The exhibition of a pesticidal mode of action either through a pro-pesticidal mechanism or maintenance of the parental toxicophore could be of lower important when considering chronic effects since pesticidal modes of action are predominantly designed to act rapidly. A complete change in mode of action could see transformation products exhibiting long-term effects on ecosystems not exhibited by the parent pesticide.

Moreover the reasoning developed in Chapter 4 will not be appropriate for explaining increases in ecotoxicity to terrestrial non-target organisms such as earthworms. In the same manner as aquatic non-target organisms, demonstrated in Chapter 4, transformation products generally exhibit an equivalent or lower toxicity to earthworms than their parent pesticides, with only 9% demonstrating increased toxicity (Sinclair and Boxall 2009). Whilst increases in hydrophobicity can explain increases in toxicity to aquatic organisms due to increased partitioning between the aqueous phase and the organism, it is not as straight forward for terrestrial organisms. Hydrophobicity is correlated to sorptive behaviour of uncharged chemicals in soil (Briggs 1981) and thereby the less hydrophobic a compound the greater the proportion will be present in the porewater and potentially bioavailable but very low hydrophobic chemicals would never reach excessive concentrations due to high elimination rates (Belfroid et al. 1995). Moreover bioavailability can be time-dependent where increased residence can exhibit decreases in bioavailability (Alexander 2000). Transformation products have limited potency to earthworms in general, however it would be useful, if suitable data were available to identify the reasoning why some compounds exhibit increased potency when compared to their parent pesticide for this taxa and other terrestrial organisms.

7.4.1.2 Estimation of environmental properties

During Chapter 3 estimation techniques were evaluated to determine their suitability at estimating physico-chemical and environmental properties of pesticides and their transformation products. Hydrophobicity and dissociation were found to be accurately estimated, soil sorption (K_{oc}) was adequately estimated, but could have been better, water solubility, vapour pressure, henry's law constant and soil persistence ($DT_{50}/t_{½}$) were poorly estimated. The environmental parameters K_{oc} and soil $DT_{50}/t_{½}$ are crucial when assessing environmental risk of anthropogenic substances.

Computational chemical scientists generally develop methodologies to estimate physico-chemical and environmental properties in the same manner, i.e. individual values for each compound are gathered into a training set and used to develop a statistical relationship, which is evaluated with a test set. Physico-chemical properties such as vapour pressure and water solubility can vary depending on the test conditions, comparable equivalent data for different compounds are simple to identify and collate, e.g. determinations at 25°C. However for environmental properties the experimental matrices are highly variable and can significantly influence the value of the parameter being determined.

When determined experimentally, K_{oc} and $DT_{50}/t_{½}$ are measured in a number of soils with differing properties, e.g. pH, % organic carbon content and % clay content, and the mean value then used for risk assessment and often used during the development of predictive approaches (e.g. Dearden 2004). The exact soils used to determine these properties can significantly influence the ultimate value(s) determined experimentally, when considering K_{oc} the organic carbon content is important for neutral compounds (Lambert et al. 1965) and alternative properties can be important for ionic compounds (Kah and Brown 2007). Guidelines suggest soils used experimentally fit specific criteria (OECD 2000) but two laboratories could still use very different soils to determine the same property for the same compound. However whilst the mean value from a number of soils will reduce the influence of soil type it will not eradicate it therefore; 1) the mean value will depend on the soils selected and 2) using the mean value in the development of predictive approaches loses a significant level of information that is particularly rich in the pesticide (and pesticide transformation product) field.

Rather than using mean values it would be pertinent to collate the substantial data that is available on K_{oc} or $DT_{50}/t_{½}$ and associated soil properties. Multiple values for some compounds linked to the soil property data could then be used for the development or refinement of predictive approaches. As a minimum this

should include clay content, pH and organic matter content. It is anticipated that there must have been hundreds and hundreds of sorption and soil degradation studies performed on pesticides and their transformation products in one or more soils. If these data were collated it is probable that an estimation methodology could be developed that is appropriate for pesticides and their transformation products and appreciably better than those methodologies currently available for these crucial parameters. When considering soil sorption this approach would be relatively straightforward but may not be so when considering soil persistence as the soil properties controlling this process are not as clear as those for sorption. However a significant dataset is also available to investigate this property and can be considered imperative as current approaches are unsuitable (Fenner et al. 2007).

7.4.1.3 Use of predictive approaches within the risk assessment framework

Predictive techniques, QSAR in particular, can be relatively simple and quick to use, even by the inexperienced. Generally all that is required is the derivation of the correct input parameter for the query molecule, be it structural, property or molecular descriptor based, it is then entered into the model/relationship and the prediction can be generated. However it is imperative that the model used is valid, applicable to the query molecule, i.e. fits within the applicability domain of the model (Jaworska et al. 2005), and is relevant for regulatory purposes. It is therefore important that predictive techniques are used cautiously by non-experts and when used the appropriateness of the model and the appropriateness of applying the model to the query molecule are documented. Currently no guidance exists when using predictive approaches for the ecotoxicological and toxicological estimation of pesticide transformation products (and impurities). Regulators currently appear to accept results from 'known' methodologies and question alternative methodologies.

Within other chemical risk assessment frameworks, e.g. REACH Directive, the use of predictive methodologies is structured requiring the development of specific documents that report on the suitability of the model itself and the

prediction generated for the query molecule. This supporting documentation are generally based on the five QSAR principles, commonly known as the 'Setubal principles' which have now been accepted by the OECD and these state a model should; 1) have a defined endpoint, 2) be based on an unambiguous algorithm; 3) have a defined domain of applicability, 4) have appropriate measures of goodness-of-fit, robustness and predictivity and 5) if possible a mechanistic interpretation. Rather than just accept the use of well known approaches, because the appropriateness of even common place methodologies can be called into question (e.g. Kaiser et al. 1999), guidance should be developed that specifies what information is required to support the submission of estimated values for pesticide transformation products.

It is anticipated that predictive techniques will never replace experimental studies for parent pesticides themselves. Estimation techniques are developed using known toxicological and ecotoxicological data and can therefore only provide estimates based on these data. They may predict extremes of a specific mode of action the extent of which has not been previously measured based extrapolation, but it would be impossible to identify significant potency based on a previously unknown mode of action. Therefore it is unlikely that pesticide regulators would (ever) accept estimated toxicological and ecotoxicological end-points for parent pesticides. Even within the REACH Directive and guidance, QSAR will not be used alone but rather in a weight of evidence approach using additional supporting data. Therefore QSAR do have a role to play during the risk assessment of pesticides providing data for transformation products and formulation impurities but their use in these field needs guidance to be developed.

7.4.2 Overall Conclusions

- When experimental data are considered transformation products are generally more hydrophilic, more water soluble and more volatile than their respective parent pesticides. Transformation products can

sometimes be more mobile and more persistent than their respective parent pesticides.

- When predictive techniques are evaluated, available approaches that estimate water solubility, vapour pressure, henry's law constant and soil degradation rate constants of transformation products perform poorly whilst acid dissociation constants using SPARC and hydrophobicity using a mean from KOWWIN, ALogPS and CLogP can be estimated accurately.

- Generally transformation products are less toxic to non-target aquatic organisms but there are occasions were they can be more toxic which can be explained by the transformation product maintaining the mode of action of the parent pesticide, a complete change in mode of action from pesticide to transformation product and/or an increase in accumulation relative to the parent pesticide. To gain a conservative estimation of transformation product ecotoxicity it is appropriate to use a battery of approaches and take the most potent valid estimate. The use of common structural moieties present within the molecules of all members of a pesticidal chemical class can be one way of determining whether a transformation product will exhibit the pesticidal mode of action of the parent pesticide.

- When the potential for pesticide transformation products to contaminate raw source dinking waters was performed for pesticides used in Great Britain transformation products from chlorpyrifos, triclopyr, trifloxystrobin, diclofop-methyl, isoproturon and propachlor were of most concern. When these were compared to another geographical area (California) different transformation products were identified as posing the greatest risk, therefore it can be concluded that it is not appropriate to use standardised determinand lists when monitoring surface waters and groundwater, site specific lists would be more appropriate.

- In general the availability of mammalian toxicity data for a range of end-points for pesticide transformation products are relatively limited. However when available experimentally determined data are examined transformation products generally exhibit a lower toxicity than their parental pesticides, most transformation products are not mutagenic and most transformation products rat oral LD_{50} can be considered of low toxicity. When these endpoints are estimated predictive toxicological approaches perform better at identifying compounds with limited toxicological concerns rather than identifying specific concerns in certain molecules. To estimate whether a transformation product exhibits mutagenicity it is most appropriate to consider parent pesticide mutagenicity together with DEREK alerts for mutagenicity and chromosome damage and TOPKAT estimates of mutagenicity. When estimating rat oral LD50 the model available in TOPKAT can provide useful data on this end-point.

7.4.3 Recommendations for further work

During this study a number of areas have been identified as requiring further study. These are detailed below:

- Degradation rate constants within environmental compartments of interest are key parameters when undertaking modelling, prioritisation and risk assessment methodologies, together with sorptive behaviour the dataset available for these parameters for pesticides and their transformation products is of the highest quality and is abundantly available (if only in summary form). Therefore it would be beneficial if these data can be used to investigate and develop high quality methods suitable for the estimation of $DT_{50}/t_{½}$ and K_{oc} for pesticide transformation products in soil.

- Estimation techniques are commonly accepted by regulators for pesticide formulation impurities as well as transformation products. Whilst this makes sense as they are all chemically/structurally related it would be prudent to evaluate that these methodologies are appropriate for this group of compounds also.

- Data are available that suggest that pesticides and transformation products can be present in raw source waters that are subsequently treated for drinking purposes. Limited studies have indicated that harsh treatments such as ozonation, chlorination and/or UV treatment can alter the structure of compounds present in the waters, sometimes to more toxic compounds. Work is required to 1) identify the fate of pesticides and transformation products during drinking water treatment, 2) identify what compounds can be formed and 3) determine whether any of these products pose a risk to consumers.

- Identification of transformation products produced following the degradation of pesticides in different systems is very complicated and very expensive. Approaches have been successfully developed to identify compounds formed in other systems e.g. mammalian metabolism. It would be advantageous if an accurate approach can be developed that provides the identity of potential transformation products in important degradation studies, i.e. soil and water/sediment systems.

- Most of the ecotoxicological work undertaken for transformation products focuses on acute aquatic end-points. However there are only limited data available on the effects these compounds may have long-term and on terrestrial organisms. Therefore further work is required to ensure that aquatic systems are not effected long-term by pesticides, transformation products and mixtures of these and that transformation products do not effect organisms residing in the terrestrial compartment.

8 Reference List

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Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Aerobic soil (laboratory)				
cis-3-chloroallyl alcohol	1,3-dichloropropene	major [g]	-	EPA 1998a
trans-3-chloroallyl alcohol	1,3-dichloropropene	major [g]	-	EPA 1998a
cis-3-chloroprop-2-enoic acid	1,3-dichloropropene	major [g]	-	EPA 1998a
trans-3-chloroprop-2-enoic acid	1,3-dichloropropene	major [g]	-	EPA 1998a
(EZ)-3-chloroacrylic acid	1,3-dichloropropene	37%	28 days	EFSA 2006a
(EZ)-3-chloroallyl alcohol	1,3-dichloropropene	1.4%	3 days	EFSA 2006a
2,4-dichlorophenol	2,4-D	3 ± 1%	8 days	Smith and Aubin 1991
		11%	-	Roberts 1998
		trace	14 days	PSD 1993a
		2-5%	10 days	PSD 1993a
2,4-dichloroanisole	2,4-D	10 ± 1%	16 days	Smith and Aubin 1991
		2-5%	10 days	PSD 1993a
2,4-D	2,4-DB	26.1%	48 days	EU 2002a
methamidophos	acephate	major [g]	-	EPA 2001a
acetochlor oxanilic acid	acetochlor	> 10%	-	Roberts 1998
2-([N-(ethoxymethyl)-N-(2-ethyl-6-methylphenyl)carbomyl]methylsulfonyl) acetic acid	acetochlor	> 10%	-	Roberts 1998
N-(ethoxymethyl)-N-(2-ethyl-6-methylphenyl)-2-sulfoneacetamide	acetochlor	> 10%	-	Roberts 1998
N-(2-ethyl-6-methylphenyl)-2-sulfoneacetamide	acetochlor	> 10%	-	Roberts 1998
2,6-diethyl-N-methoxy-methoxanilic acid	alachlor	13 - 22%	4 - 7 weeks	PSD 1990a
2,6-diethyl-N-methoxymethyl-2-sulpho-acetanilide	alachlor	15 - 25%	4 - 7 weeks	PSD 1990a
alachlor ethane sulfonic acid	alachlor	20%	9 days	Aga and Thurman 2001
		24.9% [b]	50 days	EPA 1998b
		6.5% [b]	30 days	EPA 1998b
alachlor sulfinylacetic acid	alachlor	15.9% [b]	-	EPA 1998b
		15.9 - 16.2% [b]	62 days	EPA 1998b
alachlor DM-oxanilic acid	alachlor	15.8 - 17% [b]	175 days	EPA 1998b
		14.4% [b]	62 days	EPA 1998b
alachlor oxanilic acid	alachlor	12.7 - 22.4% [b]	28 - 50 days	EPA 1998b
		9.7 - 10% [b]	20 days	EPA 1998b
2',6'-diethyl-2-hydroxy-N-methoxymethylacetanilide	alachlor	6.4 - 10.2% [b]	7 - 21 days	EPA 1998b
aldicarb sulfoxide	aldicarb	67 -92%	-	APVMA 2001
		86.1%	14 days	APVMA 2001
		70 - 90%	7 -28 days	APVMA 2001
aldicarb sulfone	aldicarb	50 - 73%	-	APVMA 2001
		80.1%	21 days	APVMA 2001
HOE 101630	amidosulfuron	7%	3 days	PSD 1994a
		5.2%	14 days	PSD 1994a
		49.6%	7 days	PSD 1994a
		40.4%	49 days	PSD 1994a
		21%	49 days	PSD 1994a
2-amino-4,6-dihydroxypyrimidine	amidosulfuron	30%	49 days	PSD 1994a
BTS 27271	amitraz	13%	-	EPA 1996a
BTS 27919	amitraz	35%	-	EPA 1996a
BTS 24868	amitraz	13%	-	EPA 1996a
dihydroxy anilazine	anilazine	19.2%	72 hours	PSD 1994b
		43%	366 days	PSD 1994b
		21%	46 hours	PSD 1994b
		0.5%	-	PSD 1994b
		9 - 12%	3 - 112 days	PSD 1994b
		13.2%	111 days	PSD 1994b
		4.6%	0 days	PSD 1994b
		6.8% (sterile)	28 days	PSD 1994b
		15.7%	2 days	PSD 1994b
		7%	100 days	PSD 1994b
sulphanilamide	asulam	3.6%	-	EPA 1995a
ionic form of asulam	asulam	22.7%	-	EPA 1995a
conjugated form of asulam	asulam	6.2%	-	EPA 1995a
conjugated acetyl asulam	asulam	trace [g]	-	EPA 1995a
conjugated acetyl sulphanilamide	asulam	trace [g]	-	EPA 1995a
methylbenzenesulfonyl carbamate	asulam	trace [g]	-	EPA 1995a
hydroxyatrazine	atrazine	19%	95 days	Assaf and Turco 1994
		0.7%	62 days	Solomon et al. 1996
		<5%	-	APVMA 1997a
deethylatrazine	atrazine	12.4%	142 days	Assaf and Turco 1994
		4.18%	244 days	Solomon et al. 1996
		8%	-	APVMA 1997a
deisopropylatrazine	atrazine	10.1%	95 days	Assaf and Turco 1994
		1.61%	244 days	Solomon et al. 1996
		<5%	-	APVMA 1997a

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Aerobic soil (laboratory) continued...				
diaminochloroatrazine	atrazine	6.7%	95 days	Assaf and Turco 1994
		0.7%	3 days	Solomon et al. 1996
		<5%	-	APVMA 1997a
DEHA	atrazine	11%	250 days	Assaf and Turco 1994
DIHA	atrazine	7.8%	250 days	Assaf and Turco 1994
azoxystrobin acid	azoxystrobin	20%	-	Roberts and Hutson 1999
reference compound 2	azoxystrobin	major [g]	-	PMRA 2000a
reference compound 3	azoxystrobin	minor [g]	-	PMRA 2000a
reference compound 10	azoxystrobin	minor [g]	-	PMRA 2000a
reference compound 20	azoxystrobin	minor [g]	-	PMRA 2000a
reference compound 28	azoxystrobin	minor [g]	-	PMRA 2000a
reference compound 36	azoxystrobin	minor [g]	-	PMRA 2000a
benalaxyl M1	benalaxyl	31%	133 days	EU 2004c
benalaxyl M2	benalaxyl	34.1%	98 days	EU 2004c
benalaxyl acid	benalaxyl	4.9%	28 days	EU 2004c
2,6-dinitro-4-trifluoromethyl-phenol	benfluralin	6%	-	EPA 2004a
carbofuran	benfuracarb	73 - 93%	0 days	PSD 1998a
carbendazim	benomyl	major [g]	-	Roberts and Hutson 1999
benzimidazole-2-ylamine	benomyl	minor [g]	-	Roberts and Hutson 1999
bensulide oxon	bensulide	13.8%	270 days	PMRA 2003e
n-methyl-bentazone	bentazone	1.7 - 4.5%	48 days	Wagner et al. 1996
5-(2,4-dichlorophenoxy)-2-nitrobenzoic acid	bifenox	principal [g]	-	Roberts 1998
methyl-5-(2,4-dichlorophenoxy)anthranilate	bifenox	principal [g]	-	Roberts 1998
bitertanol benzoic acid	bitertanol	19%	30 days	Roberts and Hutson 1999
		8.6%	29 days	PSD 1994c
bitertanol ketone	bitertanol	< 2%	-	Roberts and Hutson 1999
M510F49	boscalid	14% [b]	-	PMRA 2004e
5-bromo-6-methyluracil	bromacil	3.4% [b]	304 days	EPA 1996c
5-bromo-3-(alpha-hydroxymethylpropyl)-6-methyluracil	bromacil	1.5% [b]	154 days	EPA 1996c
5-bromo-3-sec-butyl-6-hydroxymethyluracil	bromacil	0.6% [b]	184 days	EPA 1996c
5-bromo-3-(2-hydroxy-1-methylpropyl)-6-methyluracil	bromacil	0.8% [b]	304 days	EPA 1996c
3-sec-butyl-6-methyluracil	bromacil	0.7% [b]	304 days	EPA 1996c
3,5-dibromo-4-hydroxybenzamide	bromoxynil	20.9 - 21.6% [b]	1 day	EU 2004d
		21.6% [b]	3 hours	PSD 1995l
3,5-dibromo-4-hydroxybenzoic acid	bromoxynil	16.1 - 34.8% [b]	1 day	EU 2004d
bromoxynil	bromoxynil octanoate	44.6% [b]	4 days	EU 2004d
3,5-dibromo-4-hydroxybenzamide	bromoxynil octanoate	20% [b]	28 hours	EU 2004d
RPA 401527	bromuconazole	0.02%	-	PSD 1996a
LS 860976	bromuconazole	0.09%	-	PSD 1996a
LS 860551	bromuconazole	0.03%	-	PSD 1996a
p-hydroxy buprofezin	buprofezin	< 3%	150 days	PSD 1993b
buprofezin sulphoxide	buprofezin	< 3%	150 days	PSD 1993b
buprofezin metabolite 9	buprofezin	< 3%	150 days	PSD 1993b
1-tert-butyl-3-isopropyl-5-phenyl-2-biuret	buprofezin	< 3%	150 days	PSD 1993b
1-isopropyl-3-phenyl urea	buprofezin	< 3%	150 days	PSD 1993b
DNTBA	butralin	2.2%	365 days	EPA 1998d
tetrahydrophthalamide	captan	66%	7 days	EPA 1999a
1-napthol	carbaryl	major [g]	-	EPA 2004b
		0.02%	-	Murthy and Raghu 1989
5-hydroxy carbaryl	carbaryl	2.53%	-	Murthy and Raghu 1989
4-hydroxy carbaryl	carbaryl	0.16%	-	Murthy and Raghu 1989
1-napthyl N-hydroxy methyl carbamate	carbaryl	0.2%	-	Murthy and Raghu 1989
2-chlorobenzoic acid	clofentazine	major [g]	-	Tomlin 2000
5-amino-4-chloropyridazin-3(2H)-one	chloridazon	43.2 - 46.6%	187 days	Roberts 1998
5-amino-4-chloro-2-methyl-2-hydropyridazin-3-one	chloridazon	1.2 - 1.3%	187 days	Roberts 1998
3-carbamyl-2,4,5-trichlorobenzoic acid	chlorothalonil	25%	56 days	Regitano et al. 2001
		13.2% [b]	30 days	EU 2005b
4-hydroxy-2,5,6-trichloroisophthalonitrile	chlorothalonil	< 10%	0 - 14 days	Regitano et al. 2001
		13.5%	90 days	PSD 2002

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Aerobic soil (laboratory) continued...				
		22.3%	13 weeks	PSD 2002
		32%	60 days	EPA 1999b
		32% [b]	60 days	EU 2005b
3-cyano-2,4,5,6-tetrachlorobenzamide	chlorothalonil	< 10%	0- 14 days	Regitano et al. 2001
		<10%	90 days	PSD 2002
		10.4%	13 weeks	PSD 2002
		7%	7 - 16 days	EPA 1999b
		10% [b]	7 days	EU 2005b
3-carbamyl-1,2,4,5-tetrachlorobezoic acid	chlorothalonil	4.3%	13 weeks	PSD 2002
3-cyano-6-hydroxy-2,4,5-trichlorobenzamide	chlorothalonil	3.8%	13 weeks	PSD 2002
3-cyano-2,5,6-trichlorobenzamide	chlorothalonil	3.2%	13 weeks	PSD 2002
R417888	chlorothalonil	20% [b]	62 - 181 days	EU 2005b
R417811	chlorothalonil	11% [b]	-	EU 2005b
R419492	chlorothalonil	12.4% [b]	120 days	EU 2005b
desethyl chlorfenvinphos	chlorfenvinphos	< 7%	4 months	PSD 1994d
2,4-dichlorophenyl)-ethan-1,2-diol	chlorfenvinphos	< 7%	4 months	PSD 1994d
1-(2,4-dichlorohenyl) ethan-1-ol	chlorfenvinphos	< 7%	4 months	PSD 1994d
2,4-dichloroacetophenone	chlorfenvinphos	< 7%	4 months	PSD 1994d
2,4-dichlorophenyl chloride	chlorfenvinphos	< 7%	4 months	PSD 1994d
2,4-dichlorophenyloxrane	chlorfenvinphos	< 7%	4 months	PSD 1994d
salts or conjugates desethyl chlorfenvinphos	chlorfenvinphos	< 7%	4 months	PSD 1994d
2,4-dichloro-1-(1-hydroxyethyl) benzene	chlorfenvinphos	0.4 - 6.7%	-	APVMA 2000a
3,5,6-trichloro-2-pyridinol	chlorpyrifos	29%	24 months	Baskaran et al. 1999
		18.5%	21 days	Baskaran et al. 2003
		32% [b]	365 days	EPA 1999d
		22% [b]	360 days	EPA 1999d
		0.9 -32.4%	360 days	APVMA 2000b
		30 - 38%	14 - 360 days	EU 2005d
3,5,6-trichloro-2-methoxypyridine	chlorpyrifos	< 8%	-	EPA 1999d
3,5,6-trichloro-2-pyridinol	chlorpyrifos-methyl	43% [g]	7 days	EU 2005e
2-chlorobenzene sulfonamide	chlorsulfuron	50%	2 months	PSD 1991a
3-(3-chloro-p-tolyl)-1-methylurea	chlorotoluron	30%	16 - 84 days	EU 2005c
5-chloro-3-fluoro-2-hydroxy-pyridine	clodinafop-propargyl	9 -14%	-	PSD 1995a
cloquintocet acid	cloquintocet-mexyl	<20%	-	PSD 1995a
6-hydroxyl-3-methylbenzofuran	coumaphos	0.1%	9 months	EPA 1996d
chlorfen	coumaphos	6.2%	6 months	EPA 1996d
coumaphoxon	coumaphos	0.2%	-	EPA 1996d
3-methyl-6-hydroxybenzofuran	coumaphos	4.1%	3 months	EPA 1996d
cyanazine acid	cyanazine	>50%	40 days	Blumhorst and Weber 1992
CCIM	cyazofamid	18.4 - 31.3%	3 -10 days	EU 2002e
CCIM-AM	cyazofamid	9.6 - 13.7%	7 - 10 days	EU 2002e
CTCA	cyazofamid	17.1 - 21.3%	15 - 21 days	EU 2002e
T2SO	cycloxydim	39%	7 days	PSD 1990b
$T2SO_2$	cycloxydim	3 - 4%	21 days	PSD 1990b
T2SO	cycloxydim	48%	7 days	PSD 1990b
$T2SO_2$	cycloxydim	10%	21 days	PSD 1990b
TSO2	cycloxydim	7%	43 days	PSD 1990b
T1SO	cycloxydim	3%	21 days	PSD 1990b
T1S	cycloxydim	3%	1 days	PSD 1990b
compound XV	*lambda*-cyhalothrin	12% [b]	63 days	EU 2001d
		11%	-	PMRA 2003d
compound 1a	*lambda*-cyhalothrin	7%	-	PMRA 2003d
DCVA	cyfluthrin	>10%	-	EU 2002c
4-fluoro-3-phenoxybenzoic acid	cyfluthrin	31% [b]	118 days	EU 2002c
3-phenoxybenzoic acid	alpha-cypermethrin	major [g]	-	Roberts and Hutson 1999
cyano(3-hydroxyphenyl)methyl 3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate	alpha-cypermethrin	major [g]	-	Roberts and Hutson 1999
4-hydroxy cypermethrin	alpha-cypermethrin	major [g]	-	Roberts and Hutson 1999
3-phenoxybenzoic acid	cypermethrin	23-48%	364 days	EU 2004b
		0.2-0.4%	-	Class 1992
CCA	cypermethrin	0.2-0.4%	-	Class 1992
3-phenoxybenzaldehyde	cypermethrin	0.2-0.4%	-	Class 1992
3-phenoxybenzoic acid	zeta-cypermethrin	major [g]	-	Roberts and Hutson 1999
cyano(3-hydroxyphenyl)methyl 3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate	zeta-cypermethrin	major [g]	-	Roberts and Hutson 1999

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Aerobic soil (laboratory) continued...				
4-hydroxy cypermethrin	zeta-cypermethrin	major [g]	-	Roberts and Hutson 1999
CGA 249287	cyprodinil	6%	30 days	PSD 1997a
		9%	45 days	PSD 1997a
		12%	50 days	PSD 1997a
		7.9%	21 days	PSD 1997a
melamine	cyromazine	32%	30 days	PSD 1993c
		~70%	2 - 3 weeks	PSD 1993c
		20 - 44%	29 weeks	PSD 1993c
		41%	27 weeks	PSD 1993c
formaldehyde	daminozide	trace [g]	-	EPA 1993a
methylisothiocyanate	dazomet	major [g]	-	APVMA 1997b
decamethrinic acid	deltamethrin	23% [b]	14 days	EU 2002g
ethyl-m-hydroxyphenyl carbamate	desmedipham	16%	7 days	PSD 1993d
		4.5%	14 days	PSD 1993d
		13.8% [b]	3 days	EU 2004e
		4.5% [b]	14 days	EPA 1996e
pyrimidinol	diazinon	72.9%	14 days	PSD 1991b
		2%	3 weeks	PSD 1991b
		8% (sterile)	3 weeks	PSD 1991b
hydroxyl-pyrimidinol	diazinon	1.5%	166 days	PSD 1991b
3,6-dichlorosalicylic acid	dicamba	28%	5 weeks	Smith 1973
		31%	6 weeks	Smith 1974
dimethylaminosulfanilide	dichlofluanid	major	-	HSE 2003a
methylaminosulfanilide	dichlofluanid	8.2%	97 days	HSE 2003a
2,6-dichlorobenzamide	diclobenil	13.1% [b]	50 weeks	EPA 1998e
2,4-dichlorophenol	dichlorprop	10%	8 days	Haberhauer et al. 1999
1-(2-chlorophenyl)-1-(4'-chlorophenyl)-2,2-dichloroethanol	o,p'-dicofol	major [g]	-	EPA 1998f
o,p'-dichlorobenzophenone	o,p'-dicofol	major [g]	-	EPA 1998f
2-chlorobenzoic acid	o,p'-dicofol	major [g]	-	EPA 1998f
3-hydroxy-2,4-dichlorobenzophenone	o,p'-dicofol	major [g]	-	EPA 1998f
2,4'-dichlorobenzhydrol	o,p'-dicofol	major [g]	-	EPA 1998f
1,1-(p-chlorophenyl)-2,2-dichloroethanol	p,p'-dicofol	major [g]	-	EPA 1998f
p,p'-dichlorobenzophenone	p,p'-dicofol	major [g]	-	EPA 1998f
3-hydroxy-4,4'-dichlorobenzophenone	p,p'-dicofol	major [g]	-	EPA 1998f
diclofop acid	diclofop-methyl	80 - 87%	1 day	PSD 1991c
		77%	8 days	PSD 1991c
		90%	2 days	PSD 1991c
		77.7% [b]	1 - 2 days	EPA 2000b
4-(2,4-dichlorophenoxy)phenol	diclofop-methyl	0.7 - 3%	16 days	PSD 1991c
		trace	14 days	PSD 1991c
		1 - 10%	-	PSD 1991c
		11%	8 days	PSD 1991c
		2.5%	6 days	PSD 1991c
		4% [b]	-	EPA 2000b
N,N-dimethylacetoacetamide	dicrotophos	20%	5 days	EPA 2002b
4-chlorophenyl urea	diflubenzuron	37% [h]	7 - 14 days	EPA 1997a
2,6-difluorobenzoic acid	diflubenzuron	minor	-	EPA 1997a
2,6-difluorobenzamide	diflubenzuron	minor	-	EPA 1997a
p-chloroaniline	diflubenzuron	minor	-	EPA 1997a
M9	diflufenzopyr	major	-	PMRA 1999b
N-demethyldimefuron	dimefuron	16.6 - 29.96%	93 days	PSD 1993e
compound B	dimefuron	0.5 - 2.2%	92 days	PSD 1993e
compound C	dimefuron	ND - 2.23%	92 days	PSD 1993e
compound D	dimefuron	0.32 - 2.8%	92 days	PSD 1993e
O-desmethyldimethoate	dimethoate	2.1%	-	PSD 1993f
		1.9 - 2.1%	2 days	EPA 1999e
O,O-dimethylphosphorothioic acid	dimethoate	1%	-	PSD 1993f
		0.4 - 1%	1 - 4 days	EPA 1999e
omethoate	dimethoate	6%	2 weeks	PSD 1993f
3-desmethyl dimethomorph and 4-desmethyl dimethomorph combined	dimethomorph	<0.5%	-	PSD 1994g
dinitro octyl phenol	dinocap	5.5%	30 days	PSD 1991d
disulfoton sulfone	disulfoton	35%	-	EPA 2002a
N'-(3,4-dichlorophenyl)-N-methylurea	diuron	20.9 - 22.5%	365 days	EPA 2003b
3,4-dichlorophenylurea	diuron	minor [g]	-	EPA 2003b
endosulfan sulphate	endosulfan	major [g]	-	EPA 2002c
EPTC sulfoxide	EPTC	5.6%	14 days	EPA 1999c
		≤6%	-	EPA 1999c
desphenyl-fenvalerate	esfenvalerate	0.9 - 6.4%	12 weeks	PSD 1992c
$CONH_2$-fen	esfenvalerate	1.5%	180 days	PSD 1992c
		32% [b]	12 months	PSD 1992c

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Aerobic soil (laboratory) continued...				
		1 - 4%	30 days	PSD 1992c
4'-OH-fen	esfenvalerate	1.3%	14 days	PSD 1992c
		3%	1 month	PSD 1992c
		1 - 4%	30 days	PSD 1992c
3-benzylbenzoic acid	esfenvalerate	1.4%	14 days	PSD 1992c
Cl-Vacid	esfenvalerate	3%	12 months	PSD 1992c
		1 - 4%	30 days	PSD 1992c
SD 50365	esfenvalerate	1%	3 months	PSD 1992c
		1 - 4%	30 days	PSD 1992c
triazine amine C	ethametsulfuron-methyl	major	-	PMRA 1992
ethylene	ethephon	15%	21 days	EPA 1995b
2-hydroxy ethyl phosphonic acid	ethephon	63.5%	30 days	EPA 1995b
deethyl ethirimol	ethirimol	major [g]	-	Roberts and Hutson 1999
hydroxybutyl ethirimol	ethirimol	major [g]	-	Roberts and Hutson 1999
IN-JS940	famoxadone	major [g]	-	PMRA 2003h
IN-KZ007	famoxadone	major [g]	-	PMRA 2003h
IN-MN467	famoxadone	minor [g]	-	PMRA 2003h
RH-6467	fenbuconazole	<10%	-	PSD 1995c
		<7.9%	-	PSD 1995c
		minor	-	PMRA 2003i
RH-9129	fenbuconazole	<10%	-	PSD 1995c
		major	-	PMRA 2003i
		minor	-	PMRA 2003i
RH-9130	fenbuconazole	<4.5%	-	PSD 1995c
		minor	-	PMRA 2003i
1,2,4-triazole	fenbuconazole	minor	-	PMRA 2003i
HOE 83348	fenchlorazole-ethyl	4.5%	8 days	PSD 1990e
		20%	97 days	PSD 1990e
HOE 88988	fenchlorazole-ethyl	1.5%	8 days	PSD 1990e
HOE 88989	fenchlorazole-ethyl	14.2%	8 days	PSD 1990e
		27%	97 days	PSD 1990e
HOE 72829	fenchlorazole-ethyl	2.1%	8 days	PSD 1990e
		36%	2 days	PSD 1990e
HOE 87606	fenchlorazole-ethyl	1%	8 days	PSD 1990e
HOE 87607	fenchlorazole-ethyl	11%	-	PSD 1990e
HOE 89628	fenchlorazole-ethyl	7%	97 days	PSD 1990e
3-methyl-4-nitrophenol	fenitrothion	major [g]	-	PMRA 1993a
		10 - 20%	30 days	APVMA 1999
		5 - 7%	50 days	APVMA 1999
		30%	1 - 2 weeks	APVMA 1999
		20.5%	3 days	APVMA 1999
		20% [b]	1 - 3 days	EPA 1995c
fenitrooxon	fenitrothion	0.7%	1 day	APVMA 1999
		<0.9%	21 days	EPA 1995c
desmethyl fenitooxon	fenitrothion	0.6%	1 - 5 days	APVMA 1999
		<0.9%	21 days	EPA 1995c
3-methyl-4-nitroanisole	fenitrothion	0.5%	10 days	APVMA 1999
		<0.9%	21 days	EPA 1995c
formylaminofenitrothion	fenitrothion	0.4%	10 days	APVMA 1999
4-(6-chloro-2-benzoxazolyloxy)phenol	fenoxaprop-p-ethyl	<3%	-	PSD 1990d
Ro 16-8797	fenoxycarb	<8%	-	PSD 1997b
Ro 17-3192	fenoxycarb	<8%	-	PSD 1997b
Ro 1-1374	fenoxycarb	<10%	-	PSD 1997b
α-carbomoyl-3-phenoxybenzyl-2,2,3,3-tetramethyl cyclopropane carboxylate and α-carboxy-3-phenoxybenzyl-2,2,3,3-tetramethyl cyclopropane carboxylate combined	fenpropathrin	14%	-	PSD 1989a
		7%	8 weeks	PSD 1989a
α-carboxy-3-phenoxybenzyl-2,2,3,3-tetramethyl cyclopropane carboxylate	fenpropathrin	0.3%	26 weeks	PSD 1989a
3-phenoxybenzoic acid	fenpropathrin	14%	-	PSD 1989a
		0.6%	160 days	PSD 1989a
2,2,3,3-tetramethyl cyclopropane carboxylic acid	fenpropathrin	7%	8 weeks	PSD 1989a
		<0.1%	60 days	PSD 1989a
R0 18-5445	fenpropidin	1 – 5%	-	PSD 1993g
R0 12-7124	fenpropidin	1 – 5%	-	PSD 1993g
M3	fenpyroximate	2.6 - 10.8%	14 - 28 days	PSD 1995d
		4.9 - 7.9%	16 - 32 days	PSD 1995d
1,3-dimethyl-5-phenoxypyrazole-4-carbonitrile	fenpyroximate	8.2 - 8.8%	28 days	PSD 1995d

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Aerobic soil (laboratory) continued...				
RPA 200766	fipronil	26 - 36%	-	HSE 1999
		>30 - 47%	1 year	HSE 1999
		38%	-	PSD 2004a
		57%	157 days	PSD 2004a
MB 46136	fipronil	14 - 22%	-	HSE 1999
		20 - 23.6%	-	HSE 1999
		22%	-	PSD 2004a
RPA 200761	fipronil	21%	-	PSD 2004a
MB 45950	fipronil	<5%	-	PSD 2004a
		<9%	-	PSD 2004a
		<8%	-	PSD 2004a
MB 46513	fipronil	<5%	-	PSD 2004a
		<9%	-	PSD 2004a
MB 45897	fipronil	<5%	-	PSD 2004a
		<9%	-	PSD 2004a
		<8%	-	PSD 2004a
MB 46233		<8%	-	PSD 2004a
RPA 105048	fipronil	<9%	-	PSD 2004a
RPA 105320	fipronil	<9%	-	PSD 2004a
		<8%	-	PSD 2004a
RPA 106681	fipronil	<8%	-	PSD 2004a
MB 46400	fipronil	<8%	-	PSD 2004a
flamprop-M acid	flamprop-M-isopropyl	major [g]	-	Roberts 1998
5-hydroxy-XDE-570	florasulam	72%	3 days	PMRA 2001c
		50%	14 days	PMRA 2001c
N-(2,6-difluorophenyl)-5-aminosulphonyl-1H-1,2,4-triazole-3-carboxylic acid	florasulam	18%	59 days	PMRA 2001c
5-(aminosulphonyl)-1H-1,2,4-triazole-3-carboxylic acid	florasulam	40%	59 days	PMRA 2001c
1H-1,2,4-triazole-3-sulphonamide	florasulam	16%	100 days	PMRA 2001c
N-(2,6-difluorophenyl)-1H-1,2,4-triazole-3-sulphonamide	florasulam	<4%	-	PMRA 2001c
fluazifop acid	fluazifop-butyl	major [g]	-	PMRA 1988
5-trifluoromethyl-pyrid-2-one	fluazifop-butyl	major [g]	-	PMRA 1988
fluzaifop acid	fluazifop-P-butyl	97%	2 days	PSD 1988d
		major [g]	-	PMRA 1988
5-trifluoromethyl-pryid-2-one	fluazifop-P-butyl	major [g]	-	PMRA 1988
5-trifluoromethyl-2-pyridone and 2-(4-hydroxyphenoxy)-5-trifluoromethyl pyridine combined	fluazifop-P-butyl	50%	2 - 12 weeks	PSD 1988d
compound VII	fluazinam	2.5%	90 days	PSD 1994i
		<2%	-	PSD 1994i
compound VIII	fluazinam	1.5%	30 days	PSD 1994i
		<2%	-	PSD 1994i
compound XII	fluazinam	11.4%	30 days	PSD 1994i
		7%	-	PSD 1994i
		major [g]	-	PMRA 2003j
MKH 6562 sulfonamide	flubcarbazone-sodium	46 - 69%	-	PMRA 2000c
MKH 6562 sulfonic acid	flubcarbazone-sodium	11%	-	PMRA 2000c
O-desmethyl MKH 6562	flubcarbazone-sodium	15%	-	PMRA 2000c
NMT	flubcarbazone-sodium	14.2%	-	PMRA 2000c
NODT	flubcarbazone-sodium	4.7%	-	PMRA 2000c
MKH 6562 sulfonyl urea	flubcarbazone-sodium	2%	-	PMRA 2000c
FOE sulfonic acid	flufenacet	14 - 23%	120 days	PMRA 2000d
FOE oxalte	flufenacet	10 - 16%	14 - 56 days	PMRA 2000d
FOE thioglycolate sulfoxide	flufenacet	minor [g]	-	PMRA 2000d
FOE methyl sulfoxide	flufenacet	minor [g]	-	PMRA 2000d
FOE methyl sulfone	flufenacet	minor [g]	-	PMRA 2000d
thiadone	flufenacet	minor [g]	-	PMRA 2000d
4-(2-chloro-α,α,α-trifluoro-p-tolyloxy)-2-fluorophenyl urea	flufenoxuron	9.5 - 14% [b]	30 days	HSE 1995
p-aminodiphenyl ether	flufenoxuron	0.1 - 1% [b]	-	HSE 1995
RH-5781	fluoroglycofen-ethyl	79%	21 days	PSD 1992d
RH-9985	fluoroglycofen-ethyl	8.1%	-	PSD 1992d
RH-5349	fluoroglycofen-ethyl	6%	51 days	PSD 1992d
1-(4,6-dimethoxypyrimidin-2-yl)-7-(trifluoromethyl)-1,3-dihydropyridino[2,3-d]pyrimidine-2,4-dione	flupyrsulfuron-methyl	major	-	Roberts 1998
2-sulfamoyl-6-(trifluoromethyl)pyridine-3-carboxylic acid	flupyrsulfuron-methyl	major	-	Roberts 1998
methyl 2-[(4-hydroxy-6-methoxypyrimidin-2-yl)amino]-6-(trifluoromethyl)pyridine-3-carboxylate	flupyrsulfuron-methyl	minor	-	Roberts 1998

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Aerobic soil (laboratory) continued...				
1,2,4-triazole	fluquinconazole	16.1%	365 days	PSD 1999b
		4.8 - 8%	100 days	PSD 1999b
FBC 96912	fluquinconazole	28.7%	365 days	PSD 1999b
		6.6 - 10.3%	100 days	PSD 1999b
4 amino-3,5-dichloro-6-fluoro-2-pyridinol	fluroxypyr	11.5% [b]	7 days	EU 1999
4-amino-3,5-dichloro-6-fluoromethoxypyridine	fluroxypyr	17.8% [b]	28 days	EU 1999
bis (4-fluorophenyl)methyl silanol	flusilazole	4 - 5%	52 weeks	PSD 1989b
trifluoroethanoic acid	flurtamone	9.8%	-	PSD 2000a
RE 54488	flurtamone	10.8%	-	PSD 2000a
fomesafen amino acid	fomesafen	10.2%	88 days	PSD 1995f
fomesafen amine	fomesafen	20.5%	59 days	PSD 1995f
fomesafen nitro acid	fomesafen	<1%	-	PSD 1995f
AE F130619	formasulfuron	major [g]	-	PMRA 2003k
AE F092944	formasulfuron	major [g]	-	PMRA 2003k
AE F153745	formasulfuron	minor [g]	-	PMRA 2003k
AE F148003	formasulfuron	minor [g]	-	PMRA 2003k
AE F099095	formasulfuron	minor [g]		PMRA 2003k
carbamoylphosphonic acid	foseamine-ammonium	94%	0 days	EPA 1995d
carboxylphosphonic acid	foseamine-ammonium	26%	1 month	EPA 1995d
HOE 35956	glufosinate ammonium	25 - 53%	35 days	PSD 1990f
3-methyl phosphinico-proprionic acid	glufosinate ammonium	35%	96 days	PSD 1990f
		52%	95 days	PSD 1990f
		32%	16 days	PSD 1990f
		15 - 47%	7 - 14 days	PSD 1990f
		31%	37 days	PSD 1990f
HOE 64619	glufosinate ammonium	18%	95 days	PSD 1990f
		15%	16 days	PSD 1990f
		26%	14 days	PSD 1990f
HOE 64619 [f]	3-methyl phosphinico-proprionic acid	8%	16 days	PSD 1990f
		31 - 38%	21 days	PSD 1990f
HOE 65594	glufosinate ammonium	8%	8 days	PSD 1990f
		5%		PSD 1990f
HOE 86486	glufosinate ammonium	5%	95 days	PSD 1990f
		2%	16 days	PSD 1990f
HOE 85355	glufosinate ammonium	34%	0 days	PSD 1990f
aminomethylphosphonic acid	glyphosate	26 - 29% [b]	14 days	EU 2002l
		major [g]	-	EPA 1993b
		major [g]	-	PMRA 1991c
aminomethylphosphonic acid	glyphosate trimesium	15.4% [b]	14 days	EU 2002l
1,2,4-triazole	hexaconazole	> 10%	-	PMRA 1995; PMRA 1999a
3-hydroxy-cyclohexyl-6-(dimethylamino)-1-methyl-1,3,5-triazine-2,4(1H,-3H)-dione	hexazinone	18.7%	365 days	EPA 1994a
3-(ketocyclohexyl)-6-(dimethylamino)-1-methyl-1,3,5-triazine-2,4(1H,3H)-dione	hexazinone	10.9%	365 days	EPA 1994a
Metabolite B hexazinone	hexazinone	2.3%	-	EPA 1994a
Metabolite D hexazinone	hexazinone	4.8%	-	EPA 1994a
1,5-bis(-p-tolyl)-1,4-pentadiene-3-one	hydramethylnon	25.9%	3 months	PSD 1994j
1-(2,4-dichlorophenyl)-2-imidazolylethan-1-ol	imazalil	major [g]	-	Roberts 1998
M1	imazaquin	7.6%	12 months	PSD 1993h
1-(6-chloro-pyridine-3-ylmethyl)-N-nitro-2-imino-2,3-dihydro-imidazole and 1-(6-chloro-pyridine-3-ylmethyl) imidazolidine-2,4-dione combined	imidacloprid	<1.8%	100 days	PSD 1993i
1-(6-chloro-pyridine-3-ylmethyl)-N-nitroso-2-imino-imidazolidine	imidacloprid	<1.8%	100 days	PSD 1993i
		<3%	-	PSD 1993i
		<2%	-	PSD 1993i
1-(6-chloro-pyridine-3-ylmethyl)-2-imino-imidazolidine	imidacloprid	<1.8%	100 days	PSD 1993i
		4.3%	-	PSD 1993i
		<2%	-	PSD 1993i
1-(6-chloro-pyridine-3-ylmethyl)-N-nitro guanidine and 3-(6-chloro-pyridine-3-ylmethyl) imidazolidine-2,5-dione combined	imidacloprid	<1.8%	100 days	PSD 1993i
6-chloro-nicotinic acid	imidacloprid	<1.8%	100 days	PSD 1993i
		<3%	-	PSD 1993i
1-(6-chloro-pyridine-3-ylmethyl)-N-nitro guanidine	imidacloprid	<3%	-	PSD 1993i

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Aerobic soil (laboratory) continued...				
		3.4%	-	PSD 1993i
1-(6-chloro-pyridine-3-ylmethyl)-N-nitro-2-imino-imidazollidine-5-ol	imidacloprid	<3%	-	PSD 1993i
metsulfuron-methyl	iodosulfuron-methyl	major [g]	-	PMRA 2004f
AE F059411	iodosulfuron-methyl	major [g]	-	PMRA 2004f
AE F161778	iodosulfuron-methyl	major [g]	-	PMRA 2004f
AE F145741	iodosulfuron-methyl	minor [g]	-	PMRA 2004f
AE F145740	iodosulfuron-methyl	minor [g]	-	PMRA 2004f
AE 0000119	iodosulfuron-methyl	minor [g]	-	PMRA 2004f
3,5-di-iodo-4-hydroxybenzamide	ioxynil	10.5% [b]	3 days	EU 2004g
		6.23%	1 day	PSD 1995m
3,5-di-iodo-4-hydroxybenzoic acid	ioxynil	20.4% [b]	3 days	EU 2004g
		19.67%	1 day	PSD 1995m
ioxynil	ioxynil octanoate	52.6% [b]	-	EU 2004g
3,5-di-iodo-4-hydroxybenzamide	ioxynil octanoate	15.3% [b]	-	EU 2004g
propargyl butyl carbamate	IPBC	>90%	6 hours	HSE 1994
RP 30228	iprodione	31% [b]	-	EU 2002n
		6.92% [b]	14 days	EPA 1998g
RP 36221	iprodione	17% [b]	-	EU 2002n
3,5-dichloroaniline	iprodione	9.02% [b]	30 days	EPA 1998g
RP 25040	iprodione	9.47% [b]	30 days	EPA 1998g
CA 30-0155	irgarol 1051	>10%	-	HSE 2002
desmethylisoproturon	isoproturon	14% [b]	8 days	PSD 1995g
		15.6%	4 weeks	PSD 1995g
		11%	-	PSD 1995g
3-[4-(2'-hydroxy-2'-propyl)-phenyl]-methyl urea	isoproturon	1 - 2%	-	PSD 1995g
2,6-dimethoxybenzoic acid	isoxaben	14%	118 days	Roberts 1998
3-(1-ethyl-1-methylpropyl)-4-hydroisoxazol-5-one	isoxaben	12%	118 days	Roberts 1998
demethyl isoxaben	isoxaben	11%	118 days	Roberts 1998
2-hydroxy-6-methoxybenzamide	isoxaben	3%	118 days	Roberts 1998
3-(1-ethyl-1-methylpropyl)isoxazole-5-ylamine	isoxaben	12%	118 days	Roberts 1998
RPA 202248	isoxaflutole	83 - 68.4%	-	PMRA 2000e
RPA 203328	isoxaflutole	33.7 - 55.1%	-	PMRA 2000e
kresoxim-methyl acid	kresoxim-methyl	43%	180 days	Roberts and Hutson 1999
		84%	-	PSD 1997c
		66%	-	PSD 1997c
		81%	-	PSD 1997c
		4.8% (sterile)		PSD 1997c
490M0	kresoxim-methyl	<2.5%	-	PSD 1997c
		4.4%	-	PSD 1997c
490M4	kresoxim-methyl	3.3%	-	PSD 1997c
5-oxolenacil	lenacil	7 - 9%	-	Zhang et al. 1999
α-HCH	lindane	1.62% [g]	224 days	PSD 1996e
pentachlorocyclohexane	lindane	3.84% [g]	336 days	PSD 1996e
3-(3,4-dichlorophenyl)-1-methylurea	linuron	3% [b]	120 days	EPA 1995e
3-(3,4-dichlorophenyl)-1-methoxyurea	linuron	4.3 - 5.6%	6 months	PSD 1995h
		2.1% [b]	365 days	EPA 1995e
1-(3,4-dichlorophenyl)urea	linuron	0.9 - 1.1%	6 months	PSD 1995h
		1.9% [b]	28 days	EPA 1995e
malaoxon	malathion	1.4%	< 7 days	Roberts and Hutson 1999
		0.6 - 1.4%	0 days	PSD 1995i
malathion dicarboxylic acid	malathion	62%	7 days	PSD 1995i
		19.3%	2 days	PSD 1995i
malathion monocarboxylic acids combined	malathion	7%	16 hours	PSD 1995i
malic acid and lactic acid combined	malathion	16.4%	31 days	PSD 1995i
maleic acid	maleic hydrazide	<5%	-	EPA 1994b
maleimide	maleic hydrazide	<5%	-	EPA 1994b
ethylenethiourea	mancozeb	3.1% [b]	-	EU 2005h
ethyleneurea	mancozeb	8.5% [b]	-	EU 2005h
ethylenebisisothiocyanide sulfide	mancozeb	8.2% [b]	-	EU 2005h
ethylenethiourea	maneb	9.6 - 20.4%	-	EU 2005i
ethyleneurea	maneb	36.1 - 63.8%	-	EU 2005i
ethylenebisisothiocyanide sulfide	maneb	4.1 - 12.8%	-	EU 2005i
4-chloro-2-methyl phenol	mecoprop	2 - 3%	20 days	PSD 1994k
		3.5% [b]	-	EU 2003j
4-chloro-2-methyl phenol	mecoprop-P	2 - 3%	20 days	PSD 1994l
		1.95%	16 days	EU 2003k
2-methyl-4-chlorophenol	MCPA	minor [g]	-	EU 2005j
MCPA	MCPA-thioethyl	66% [b]	2 days	EU 2005j
2-methyl-4-chlorophenol	MCPA-thioethyl	19.8% [b]	12 days	EU 2005j

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Aerobic soil (laboratory) continued...				
MCPA	MCPB	6.2% [b]	8 days	EU 2005k
hydroxyMCPA	MCPB	9.5% [b]	8 days	EU 2005k
HOE 113225	mefenpyr-diethyl	42.6%	2 days	PSD 1999a
		44.1%	4 days	PSD 1999a
		46.7%	3 days	PSD 1999a
HOE 094270	mefenpyr-diethyl	50%	16 days	PSD 1999a
		72.2%	64 days	PSD 1999a
		34.9%	63 days	PSD 1999a
HOE 109453	mefenpyr-diethyl	4.9%	63 days	PSD 1999a
N-methylpiperidine	mepiquat chloride	<5%	-	EPA 1997b
piperidine	mepiquat chloride	<5%	-	EPA 1997b
CGA-62826	metalaxyl	50%	21 days	Roberts and Hutson 1999
		53.6%	66 days	EPA 1994c
acetaldehyde	metaldehyde	5%	-	PSD 1996b
paraldehyde	metaldehyde	0.4%	-	PSD 1996b
methylisothiocyanate	metam-sodium	75%	-	APVMA 1997b
metazachlor oxalic acid	metazachlor	major [g]	-	Tomlin 2000
metazachlor sulfonic acid	metazachlor	major [g]	-	Tomlin 2000
amino-N-benzothiazol-2-yl-N-methylamide	methabenzthiazuron	major [g]	-	Roberts 1998
N-benzothiazol-2-yl(methylamino)carboxamide	methabenzthiazuron	minor [g]	-	Roberts 1998
methiocarb phenol	methiocarb	2% [b]	0 days	PSD 1998b
methiocarb sulfoxide	methiocarb	30% [b]	29 days	PSD 1998b
methiocarb sulfoxide phenol	methiocarb	18% [b]	64 days	PSD 1998b
methiocarb sulfone	methiocarb	1% [b]	29 days	PSD 1998b
methiocarb sulfone phenol	methiocarb	9% [b]	91 days	PSD 1998b
methiocarb sulfone quinone	methiocarb	8% [b]	217 days	PSD 1998b
methiocarb metabolite A	methiocarb	1% [b]	29 days	PSD 1998b
S-methyl-N-hydroxythioacetimidate	methomyl	≤2%	-	EPA 1998h
RH-113154	methoxyfenozide	3.2%	-	PMRA 2004g
ethylenethiourea	metiram	12% [g]	4 days	EU 2005l
ethylenebisisothiocyanide sulfide	metiram	57% [b]	0 days	EU 2005l
carbimid	metiram	14.9% [b]	0 days	EU 2005l
TDIT	metiram	13.5% [b]	0 days	EU 2005l
metolachlor oxanilic acid	metolachlor	28.09%	90 days	EPA 1995f
CGA-37735	metolachlor	14.85%	272 days	EPA 1995f
CGA-41638	metolachlor	2.06%	90 days	EPA 1995f
CGA-13656	metolachlor	1.02%	0 days	EPA 1995f
metolachlor ethane sulfonic acid	metolachlor	5%	14 days	Aga and Thurman 2001
carbinol	metolachlor	24.3%	120 days	Rice et al. 2002
morpholinone	metolachlor	2.9%	120 days	Rice et al. 2002
ATSA	metosulam	27.7% [b]	-	PSD 1996c
7-hydroxymetosulam	metosulam	21.8% [b]	-	PSD 1996c
5-hydroxymetosulam	metosulam	5.7% [b]	-	PSD 1996c
deaminated diketo metribuzin	metribuzin	major [g]	-	EPA 1998i
diketo metribuzin	metribuzin	major [g]	-	EPA 1998i
deaminated metribuzin	metribuzin	minor [g]	-	EPA 1998i
2-methyl-deaminated diketo metribuzin	metribuzin	minor [g]	-	EPA 1998i
4-methyl-deaminated diketo metribuzin	metribuzin	minor [g]	-	EPA 1998i
3-amino-deaminated metribuzin	metribuzin	minor [g]	-	EPA 1998i
IN-D5119	metsulfuron-methyl	16%	24 weeks	PSD 1991e
		19% (sterile)	-	PSD 1991e
		8 - 29%	8 weeks	PSD 1991e
		16% [b]	24 weeks	EU 2000c
IN-D5803	metsulfuron-methyl	17% [b]	14 weeks	EU 2000c
IN-B5685	metsulfuron-methyl	17% [b]	14 weeks	EU 2000c
IN-A4098	metsulfuron-methyl	33% [b]	12 weeks	EU 2000c
IN-NC148	metsulfuron-methyl	16% [b]	12 weeks	EU 2000c
O-desmethyl metsulfuron	metsulfuron-methyl	11% [b]	10 days	EU 2000c
methyl-2-(aminosulfonyl)benzoate	metsulfuron-methyl	2 - 14%	-	PSD 1991e
		38 - 51% (sterile)	24 weeks	PSD 1991e
		6 - 9%	2 weeks	PSD 1991e
saccharin	metsulfuron-methyl	32%	16 weeks	PSD 1991e
		4 - 7% (sterile)	-	PSD 1991e
		16 - 32%	2 - 4 weeks	PSD 1991e
		47% [b]	8 weeks	EU 2000c
molinate sulfoxide	molinate	1.91% [b]	30 days	EU 2003m
hexamethyleneimine	molinate	0.66% [b]	30 days	EU 2003m
1,2,4-triazole	myclobutanil	major [g]	-	PMRA 1993b
HMUD	nicosulfuron	6.5 - 18.5% [g]	0 - 182 days	PSD 2000c
		12.9% [g]	31 days	PSD 2000c
		14.4% [g]	28 days	PSD 2000c

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Aerobic soil (laboratory) continued...				
ADMP	nicosulfuron	13 - 26.9% [g]	0 - 182 days	PSD 2000c
		7.2% [g]	31 days	PSD 2000c
ASDM	nicosulfuron	85.2% [g]	148 days	PSD 2000c
		21.5% [g]	85 days	PSD 2000c
AUSN	nicosulfuron	26.8% [g]	238 days	PSD 2000c
UCSN	nicosulfuron	11% [g]	238 days	PSD 2000c
IN-V9367	nicosulfuron	>80%	-	PMRA 1996a
IN-J290	nicosulfuron	>80%	-	PMRA 1996a
desmethyl norflurazon	norflurazon	31 - 36%	365 days	EPA 1996f
demethylomethoate and (2-methylamino-2-oxoethyldithio)acetic acid	omethoate	4.9%	-	PSD 1993j
phosphonothioacetic acid	omethoate	6.3%	49 days	PSD 1993j
2,2-dithiobis (N-methylacetamide)	omethoate	2.4%	-	PSD 1993j
N-methyl-2-methylsulfonyl-acetamide	omethoate	2.6%	-	PSD 1993j
4-hydroxy-3,5-dinitro-benzenesulfonamide	oryzalin	4.7%	1 month	EPA 1994d
		4.7%	23 days	EPA 1994d
2-ethyl-7-nitro-1-propyl-1H-benzimidazole-5-sulfonamide-3-oxide	oryzalin	2.1%	23 days	EPA 1994d
3,3'-azoxybis[4-(propylamino)-5-nitro] benzenesulfonamide	oryzalin	1.4%	23 days	EPA 1994d
3,5-dinitro-4-(propylamino) benzenesulfonamide	oryzalin	1.2%	23 days	EPA 1994d
oxadixyl acid	oxadixyl	main [g]	-	Tomlin 2000
oxamyl oxime	oxamyl	major [g]	-	EPA 2000a
dimethyloxamic acid	oxamyl	major [g]	-	EPA 2000a
ketone metabolite	paclobutrazol	18% [b]	-	PSD 1995j
4-chlorobenzylamine	pencycuron	major [g]	-	Roberts and Hutson 1999
4-chlorobenzylformamide	pencycuron	major [g]	-	Roberts and Hutson 1999
2,6-dinitro-3,4-xylidine	pendimethalin	minor [g]	-	EPA 1997d
4-[(1-ethylpropyl)amino]-2-methyl-3,5-dinitro benzyl alcohol	pendimethalin	minor [g]	-	EPA 1997d
4-[(1-ethylpropyl)amino]-3,5-dinitro-o-toluic acid	pendimethalin	minor [g]	-	EPA 1997d
phorate sulfoxide	phorate	major [g]	-	PMRA 2003a
phorate sulfone	phorate	major [g]	-	PMRA 2003a
MHPC	phenmedipham	54% [b]	5 days	EU 2004i
APMP	phenmedipham	4% [b]	56 days	EU 2004i
CL 153815	picolinafen	major [g]	-	PMRA 2003m
4-fluoroaniline	picolinafen	minor [g]	-	PMRA 2003m
dichlorobenzoic acid	piperalin	21%	14 days	EPA 1994e
3-(2-methylpiperi-dino) propyl alcohol	piperalin	10.7%	3 days	EPA 1994e
5,6-dimethyl-2-dimethylamino-pyrimidin-4-ol	pirimicarb	30 - 36%	-	PSD 1994m
5,6-dimethyl-2-methylamino-4-pyrimidin-4-ol	pirimicarb	10 - 30%	-	PSD 1994m
5,6-dimethyl-2-methylamino-pyrimidin-4-yl-dimethylcarbamate	pirimicarb	10 - 30%	-	PSD 1994m
2-diethylamino-6-methylpyrimidin-4-ol	pirimiphos-methyl	36 - 56%	2 weeks	PSD 1997d
		72 - 75%	-	PSD 1997d
O,2-diethylamino-6-methylpyrimidin-4-yl-O,O-dimethyl phosphate	pirimiphos-methyl	< 4.1%	-	PSD 1997d
2-ethylamino-6-methylpyrimidin-4-ol	pirimiphos-methyl	< 4.1%	-	PSD 1997d
		1 - 3%	-	PSD 1997d
N,N-diethylguanidine	pirimiphos-methyl	12.8 - 35.1%	-	PSD 1997d
2-amino-6-methylpyrimidin-4-ol	pirimiphos-methyl	1 - 3%	-	PSD 1997d
CGA-171683	primisulfuron methyl	88.6%	-	PMRA 2001a
saccharin	primisulfuron methyl	23.1%	-	PMRA 2001a
CGA-191429	primisulfuron methyl	14.6%	-	PMRA 2001a
CGA-177288	primisulfuron methyl	6.7%	-	PMRA 2001a
CGA-120844	primisulfuron methyl	3.9%	-	PMRA 2001a
prochloraz-formylurea	prochloraz	0.3%	-	Höllrigl-Rosta et al. 1999
prochloraz-urea	prochloraz	0.2%	-	Höllrigl-Rosta et al. 1999
2,4-bis(isopropylamino)-6-hydroxy-s-triazine	prometryn	26.2%	360 days	EPA 1996g
2-amino-4-isopropylamino-6-methylthio-s-triazine	prometryn	1.1%	30 days	EPA 1996g
RH24644	pronamide	27%	-	EPA 1994f

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Aerobic soil (laboratory) continued...				
RH24580	pronamide	14%	-	EPA 1994f
RH26521	pronamide	4%	-	EPA 1994f
propachlor oxanilic acid	propachlor	33.3%	1 month	EPA 1998j
propachlor ethane sulfonic acid	propachlor	19.1%	1 month	EPA 1998j
propachlor sulfinylacetic acid	propachlor	6.7%	1 month	EPA 1998j
hydroxypropachlor	propachlor	6%	5 days	EPA 1998j
propachlor methyl sulfone	propachlor	3.2%	4 months	EPA 1998j
norchloropropachlor	propachlor	1.2%	-	EPA 1998j
Ro 17-3102	propaquizafop	25.9 - 38.8%	1 month	PSD 1994n
		2.8 - 9% (sterile)	1 month	PSD 1994n
Ro 16-1976	propaquizafop	2.7 - 4.7%	1 month	PSD 1994n
Ro 40-2724	propaquizafop	6.5 - 16.1%	1 month	PSD 1994n
1,2,4-triazole	propiconazole	24 - 43%	-	EU 2003n
CGA 118 245	propiconazole	22%	-	EU 2003n
propylene urea	propineb	40% [b]	2 days	EU 2003o
2-(3,5-dichlorophenyl)-4,4-dimethyl-5-methyleneoxazoline	propyzamide	9%	-	Roberts 1998
		11 - 21%	60 - 90 days	EU 2003q
		10.4 - 31.9%	21 - 45 days	EU 2003q
N-(1,1-dimethylacetonyl)-3,5-dichlorobenzamide	propyzamide	77%	-	Roberts 1998
		4.5 - 30.2%	21 - 120 days	EU 2003q
[2-(3,5-dichlorophenyl)-4,4-dimethyl-1,3-oxazolin-5-ylidene]methan-1-ol	propyzamide	0.1 -1.6%	-	Roberts 1998
(3,5-dichlorophenyl)-N-(3-hydroxy-1,1-dimethyl-2-oxopropyl)carboxamide	propyzamide	0.1 -1.6%	-	Roberts 1998
(3,5-dichlorophenyl)-N-(3-hydroxy-1,1-dimethylpropyl)carboxamide	propyzamide	0.1 -1.6%	-	Roberts 1998
(3,5-dichlorophenyl)-N-(2,3-dihydroxy-1,1-dimethylpropyl)carboxamide	propyzamide	0.1 -1.6%	-	Roberts 1998
3-[(3,5-dichlorophenyl)carbonylamino]-3-methylbutanoic acid	propyzamide	0.1 -1.6%	-	Roberts 1998
2-[(3,5-dichlorophenyl)carbonylamino]-2-methylpropanoic acid	propyzamide	0.1 -1.6%	-	Roberts 1998
3-[(3,5-dichlorophenyl)carbonylamino]-3-methyl-2-oxobutanoic acid	propyzamide	0.1 -1.6%	-	Roberts 1998
CGA 180777	pymetrozine	16.5%	-	PMRA 2002
CGA 359009	pymetrozine	7.7%	-	PMRA 2002
CGA 319251	pymetrozine	0.5%	-	PMRA 2002
CGA 294849	pymetrozine	7%	-	PMRA 2002
CGA 215525	pymetrozine	3.45%	-	PMRA 2002
GS23199	pymetrozine	7.3%	-	PMRA 2002
CGA 249257	pymetrozine	<2%	-	PMRA 2002
pymetrozine metabolite VI	pymetrozine	5.2%	-	PMRA 2002
BF 500-3	pyraclostrobin	18%	-	PMRA 2003n
BF 500-6	pyraclostrobin	18%	-	PMRA 2003n
BF 500-5	pyraclostrobin	minor [g]	-	PMRA 2003n
BF 500-7	pyraclostrobin	minor [g]	-	PMRA 2003n
6-chloro-3-phenyl-pyridazin-4-ol	pyridate	88% [b]	3 days	EU 2001e
ZK 512723	pyrimethanil	8% [b]	62 days	PSD 1995k
		52 - 56%	186 - 243 days	PSD 1995k
BH518-2	quinmerac	<4%	211 days	PSD 1998c
		42.4%	224 days	PSD 1998c
BH518-1	quinmerac	<4%	211 days	PSD 1998c
		6%	-	PSD 1998c
BH518-4	quinmerac	<4%	211 days	PSD 1998c
		1 - 4%	90 days	PSD 1998c
		6%	-	PSD 1998c
BH518-5	quinmerac	<4%	365 days	PSD 1998c
		26.4%	196 days	PSD 1998c
3-hydroxuquioxyfen	quinoxyfen	<8%	-	Roberts and Hutson 1999
5,7-dichloro-4-hydroxyquinoline	quinoxyfen	6% [g]	-	Roberts and Hutson 1999
quizalofop acid	quizalofop-methyl	36%	15 days	PSD 1987
IN-70941	rimsulfuron	30.3 - 33.1%	365 days	PSD 1996f
IN-70942	rimsulfuron	20.2 - 23.5%	365 days	PSD 1996f
IN-E9260	rimsulfuron	16.3%	365 days	PSD 1996f
IN-J290	rimsulfuron	0.9%	365 days	PSD 1996f
IN-T5831	rimsulfuron	0.5%	365 days	PSD 1996f
deisopropylatrazine	simazine	10.9% [d]	30 days	PSD 1992e

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Aerobic soil (laboratory) continued...				
		3% (sterile)	3 months	PSD 1992e
		3.9%	3 months	PSD 1992e
		4.6 - 4.8%	294 days	PSD 1992e
deisopropyl hydroxyatrazine	simazine	2.4% (sterile)	3 months	PSD 1992e
		1.3%	3 months	PSD 1992e
hydroxysimazine	simazine	2.2% (sterile)	3 months	PSD 1992e
		5.6%	3 months	PSD 1992e
		<0.1 - 11%	294 days	PSD 1992e
		4%	365 days	PSD 1992e
diaminochlorotriazine	simazine	1.4% [b]	365 days	PSD 1992e
sulphonamide	sulfosulfuron	12.8% [b]	-	PMRA 1998
aminopyrimidine	sulfosulfuron	10.6% [b]	-	PMRA 1998
sulfosulfuron desmethyl	sulfosulfuron	5.2% [b]	-	PMRA 1998
sulfosulfuron guanidine	sulfosulfuron	minor [g]	-	PMRA 1998
anilino acid	tau-fluvalinate	5% [b]	-	PSD 1997e
		<9%	-	PSD 1997e
		14% [b] (sterile)	-	PSD 1997e
		9% [b]	14 days	PSD 1997e
haloaniline	tau-fluvalinate	3% [b]	-	PSD 1997e
		10% [b]	-	PSD 1997e
		4% [b] (sterile)	-	PSD 1997e
		6% [b]	30 days	PSD 1997e
dicarboxylic acid	tau-fluvainate	3% [b]	30 days	PSD 1997e
3-phenoxybenzoic acid	tau-fluvalinate	2% [b]	7 days	PSD 1997e
3-phenoxybenzaldehyde	tau-fluvalinate	1% [b]	0 days	PSD 1997e
1,2,4-triazole	tebuconazole	<0.1%	-	PSD 1993k
		3 - 6%	123 days	PSD 1993k
SN 320-1	tebuconazole	<5%	-	PSD 1993k
SN 3678-7/A	tebuconazole	<5%	-	PSD 1993k
SN 3678-7/B	tebuconazole	<5%	-	PSD 1993k
SN 320-1, SN 3678-7/A and SN 3678-7/B combined	tebuconazole	1 - 2%	123 days	PSD 1993k
RH-6595	tebufenozide	minor [g]	-	PMRA 1996b
RH-2703	tebufenozide	minor [g]	-	PMRA 1996b
RH-2651	tebufenozide	minor [g]	-	PMRA 1996b
CL 810 721	tebufenpyrad	<7%	-	PSD 1995o
N-[5-(1,1-dimethylethyl)-1,3,4-thiadiazol-2-yl]-N-methylurea	tebuthiuron	6.9%	9 months	EPA 1994g
3,4-dichloro-2,4-difluoroaniline	tebflubenzuron	5.4%	-	PSD 1991g
3,5-dichloro-2,4-difluorophenyl urea	tebflubenzuron	10.4%	-	PSD 1991g
2,3,5,6-tetrachloroaniline	tecnazene	7.4% [g]	28 days	PSD 1995p
2,3,5,6-tetrafluoro-4-methylbenzoic acid	tefluthrin	2.1% [b]	62 days	PSD 1991h
		10% [b]	122 days	PSD 1991h
2,3,5,6-tetrafluoro-1,4-benzene dicarboxylic acid	tefluthrin	1.3% [b]	180 days	PSD 1991h
tefluthrin compound V	tefluthrin	1% [b]	30 days	PSD 1991h
PP890	tefluthrin	7%	31 days	PSD 1991h
DP-1	tepraloxydim	2.8%	-	PMRA 2004b
DP-2	tepraloxydim	7.5 - 9.2%	-	PMRA 2004b
DP-4	tepraloxydim	2.4%	-	PMRA 2004b
2-hydroxy terbutryn	terbutryn	major	-	Roberts 1998
thiomethylol terbutryn	terbutryn	major	-	Roberts 1998
hydroxy-N-deethylated terbutryn	terbutryn	minor	-	Roberts 1998
thiomethylol deethylated terbutryn	terbutryn	minor	-	Roberts 1998
deethylterbuthylazine	terbuthylazine	<5%	-	Roberts 1998
1,2,4-triazole	tetraconazole	<1.7%	-	PSD 1999c
triazolylacetic acid	tetraconazole	3.55% [b]	100 days	PSD 1999c
tetraconazole acid	tetraconazole	~80%	7 days	PSD 1999c
tetraconazole alcohol	tetraconazole	<5%	-	PSD 1999c
2-ester-3-sulfonamide	thifensulfuron-methyl	6 - 11%	-	PSD 1991l
thifensulfuron acid	thifensulfuron-methyl	25%	-	EU 2001g
O-desmethyl-thifensulfuron-methyl	thifensulfuron-methyl	15%	-	EU 2001g
		14 - 19%	-	PSD 1991l
thiophene sulfonimide	thifensulfuron-methyl	<10%	52 weeks	EU 2001g
		21 - 29%	-	PSD 1991l
4-chlorobezoic acid	thiobencarb	5%	-	EPA 1997e
methomyl	thiodicarb	81.3% [b]	7 days	PSD 1992f
		79.6%	7 days	EPA 1998k
methomyl oxime	thiodicarb	2.1% [b]	3 days	PSD 1992f
methomyl sulfone	thiodicarb	minor [g]	-	PSD 1992f
methomyl oxime sulfone	thiodicarb	minor [g]	-	PSD 1992f
methomyl sulfoxide	thiodicarb	minor [g]	-	PSD 1992f
methomyl oxime sulfoxide	thiodicarb	minor [g]	-	PSD 1992f
acetonitrile	thiodicarb	minor [g]	-	EPA 1998k
carbendazim	thiophanate-methyl	41.8%	30 days	EPA 2001c
		76%	3 weeks	EPA 2001c

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Aerobic soil (laboratory) continued...				
		primary [g]	-	EPA 2004c
		62.8 - 75.8% [b]	3 - 7 days	EU 2005m
DX-105	thiophanate-methyl	<10%	-	EPA 2001c
FH-432	thiophanate-methyl	<10%	-	EPA 2001c
TM-CH2OH	tolclofos-methyl	0.4% [b]	90 days	PSD 1993l
TM-COOH	tolclofos-methyl	0.5% [b]	90 days	PSD 1993l
TMO	tolclofos-methyl	1.2% [b]	90 days	PSD 1993l
TMO-CH2OH	tolclofos-methyl	0.3% [b]	30 days	PSD 1993l
TMO-COOH	tolclofos-methyl	0.3% [b]	180 days	PSD 1993l
DM-TM	tolclofos-methyl	10.5% [b]	90 days	PSD 1993l
DM-TMO	tolclofos-methyl	3.4% [b]	180 days	PSD 1993l
ph-CH3	tolclofos-methyl	4.1% [b]	90 days	PSD 1993l
ph-CH2OH	tolclofos-methyl	0.4% [b]	180 days	PSD 1993l
ph-COOH	tolclofos-methyl	0.4% [b]	45 days	PSD 1993l
DMST	tolyfluanid	~60% [b]	-	PSD 1995q
RNH 0189	tolyfluanid	<5%	-	PSD 1995q
RNH 0166	tolyfluanid	<5%	-	PSD 1995q
RNH 0416	tolyfluanid	<5%	-	PSD 1995q
tralkoxydim metabolite 9	tralkoxydim	5.1% [c]	7 days	PSD 1993m
		29.5% [b] (sterile)	30 days	PSD 1993m
tralkoxydim metabolite 8	tralkoxydim	11.8% [b]	61 days	PSD 1993m
tralkoxydim metabolite 10	tralkoxydim	11.3% [b]	0 days	PSD 1993m
CGA 150829	triasulfuron	30% [b]	28 weeks	EU 2000d
		9.9%	116 days	PSD 1992g
CGA 195660	triasulfuron	2.4%	52 weeks	PSD 1992g
		10.4%	42 weeks	PSD 1992g
CGA 161149	triasulfuron	9.5%	8 weeks	PSD 1992g
O-desmethyl triasulfuron	triasulfuron	<10.2%	-	EU 2000d
triazamate metabolite II	triazamate	91% [b]	1 day	PSD 1998d
		71 - 75%	1 day	PSD 1998d
triazamate metabolite III	triazamate	37% [b]	2 days	PSD 1998d
		27% [b]	4 days	PSD 1998d
triazamate metabolite IV	triazamate	33 - 40% [b]	10 - 14 days	PSD 1998d
		40 - 50% [b]	101 days	PSD 1998d
triazamate metabolite IX	triazamate	39% [b]	42 days	PSD 1998d
triazamate metabolite VIII	triazamate	9 - 12% [b]	368 days	PSD 1998d
		<4%	-	PSD 1998d
SAS 9256	triazoxide	21% [b]	64 days	PSD 1993n
SAS 9709	triazoxide	7% [b]	365 days	PSD 1993n
triazine amine A	tribenuron methyl	91.1% [b]	14 days	PSD 1992h
		83% [g]	30 days	EFSA 2004
O-demethyl triazine amine A	tribenuron methyl	5.4% [b]	9 days	PSD 1992h
IN-A4098	tribenuron methyl	7.8% [b]	112 days	PSD 1992h
		13% [g]	118 days	EFSA 2004
saccharin	tribenuron-methyl	11[g]	7 days	EFSA 2004
3,5,6-trichloro-2-pyridinol	triclopyr	major [g]	-	PMRA 1991b
		26%	<30 days	EPA 1998l
3,5,6-trichloro-2-methoxypyridine	triclopyr	8%	<30 days	PMRA 1991b
CGA-321113	trifloxystrobin	major [g]	-	PMRA 2004h
CGA-357276	trifloxystrobin	minor [g]	-	PMRA 2004h
CGA-373466	trifloxystrobin	minor [g]	-	PMRA 2004h
CGA-357261	trifloxystrobin	minor [g]	-	PMRA 2004h
CGA-331409	trifloxystrobin	minor [g]	-	PMRA 2004h
CGA357262	trifloxystrobin	minor [g]	-	PMRA 2004h
NOA 413161	trifloxystrobin	minor [g]	-	PMRA 2004h
2,6-dinitro-4-(trifluoromethylphenyl)amine	trifluralin	0.2%	-	Roberts 1998
[2,6-dinitro-4-(trifluoromethyl)phenyl]propylamine	trifluralin	1.7%	1 year	Roberts 1998
α,α,α-trifluoro-2,6-dinitro-N-propyl-p-toluidine	trifluralin	2.8 - 4.6%	-	EPA 1996h
α,α,α-trifluoro-5-nitro-4-propyl-toluene-3,4-diamine	trifluralin	1.5 - 2.1%	-	EPA 1996h
2-ethyl-7-nitro-1-propyl-5-(trifluoromethyl) benzimidazole-3-oxide	trifluralin	0.1 - 0.3%	-	EPA 1996h
2-ethyl-7-nitro-1-propyl-5-(trifluoromethyl) benzimidazole	trifluralin	0.5 - 1.0%	-	EPA 1996h
2-ethyl-7-nitro-5-(trifluoromethyl) benzimidazole	trifluralin	2.1 - 2.6%	-	EPA 1996h
α,α,α-trifluoro-2,6-dinitro-p-cresol	trifluralin	0.1 - 2.7%	-	EPA 1996h
2,2'-azoxybis (α,α,α-trifluoro-6-nitro-N-propyl-p-toluidine	trifluralin	0.8 - 3.0%	-	EPA 1996h
methyl saccahrin	triflusulfuron-methyl	84% [b]	29 days	PSD 1995r
		19.9%	368 days	PMRA 1999c
N,N-bis demethyl triazine amine B	triflusulfuron-methyl	<20%	-	PSD 1995r
		10 - 13%	14 days	PMRA 1999c

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Aerobic soil (laboratory) continued...				
N-demethyl triazine amine B	triflusulfuron-methyl	<40%	-	PSD 1995r
		23.4%	368 days	PMRA 1999c
triazine amine B	triflusulfuron-methyl	<60%	-	PSD 1995r
		39% [b] (sterile)	7 days	PSD 1995r
		55.2%	21 days	PMRA 1999c
trinexapac acid	trinexapac ethyl	major [g]	-	PSD 1995s
		major [g]	-	PMRA 2001b
RPA 406341	triticonazole	10.6% [b]	112 days	PSD 2000d
		15.3% [b]	357 days	PSD 2000d
		16.1% [b]	306 days	PSD 2000d
		14.8% [b]	56 days	PSD 2000d
		10.7% [b]	8 months	PSD 2000d
		20.2%	240 days	PSD 2000d
		15.3%	-	PMRA 2000f
		3 - 15%	-	PMRA 2004c
RPA 404886	triticonazole	<6.7%	-	PSD 2000d
		minor [g]	-	PMRA 2000f
RPA 406780	triticonazole	9.4% [b]	-	PSD 2000d
		12.8% [b]	363 days	PSD 2000d
		9.9%	-	PMRA 2000f
		3 - 10%	-	PMRA 2004c
RPA 407922	triticonazole	12.8%	266 days	PSD 2000d
		10.5 -11.1% [b]	363 days	PSD 2000d
		11.5%	-	PMRA 2000f
		12%	-	PMRA 2004c
RPA 404766	triticonazole	9.5% [b]	12 months	PSD 2000d
		8.7% [b]	100 days	PSD 2000d
		9.5%	-	PMRA 2000f
		9.5% [b]	-	PMRA 2004c
RPA 406203	triticonazole	<4%	-	PSD 2000d
dihydroxy tritconazole	triticonazole	<2%	-	PSD 2000d
triticonazole metabolite 8	triticonazole	<2%	-	PSD 2000d
RH-139432	zoxamide	major [g]	-	PMRA 2001d
RH-127450	zoxamide	major [g]	-	PMRA 2001d
Anaerobic soil (laboratory)				
(EZ)-3-chloroacrylic acid	1,3-dichloropropene	55%	28 days	EFSA 2006a
(EZ)-3-chloroallyl alcohol	1,3-dichloropropene	2.6%	3 days	EFSA 2006a
2,4-D	2,4-DB	26%	31 days	EU 2002a
3-phenoxybenzoic acid	alpha-cypermethrin	67.6%	120 days	EU 2004b
dihydroxy anilazine	anilazine	36%	60 days	PSD 1994b
		35.7%	60 days	PSD 1994b
sulphanilamide	asulam	major [g]	-	EPA 1995a
acetyl asulam	asulam	14.3%	7 days	EPA 1995a
deethylatrazine	atrazine	2.1%	32 days	Solomon et al. 1996
hydroxyatrazine	atrazine	0.4%	94 days	Solomon et al. 1996
deisopropylatrazine	atrazine	0.7%	32 days	Solomon et al. 1996
diaminochloroatrazine	atrazine	0.3%	32 days	Solomon et al. 1996
reference compound 2	azoxystrobin	major [g]	-	PMRA 2000a
benalaxyl M1	benalaxyl	50.73%	203 days	EU 2004c
LS 871387	bromuconazole	10.1%	6 months	PSD 1996a
cyclohex-4-ene-2-cyano-1-carboxylic acid	captan	20%	-	EPA 1999a
1-napthol	carbaryl	0.04%	-	Murthy and Raghu 1989
5-hydroxy carbaryl	carbaryl	11.17%	-	Murthy and Raghu 1989
4-hydroxy carbaryl	carbaryl	11.11%	-	Murthy and Raghu 1989
1-napthyl N-hydroxy methyl carbamate	carbaryl	1.74%	-	Murthy and Raghu 1989
4-hydroxy-2,5,6-trichloroisophthalonitrile	chlorothalonil	17.7 - 42.8%	-	PSD 2002
		43% [b]	-	EU 2005d
3,5,6-trichloro-2-pyridinol	chlorpyrifos	major [g]	-	PSD 1999a
		>90%	270 days	EU 2005d
CCIM	cyazofamid	27.2% [g]	7 days	EU 2002e
CCIM-AM	cyazofamid	14.1% [g]	7 days	EU 2002e
CTCA	cyazofamid	21.3%	56 days	EU 2002e
4-fluoro-3-phenoxybenzoic acid	cyfluthrin	19% [b]	30 days	EU 2002c
compound Ia	cyhalothrin and *lambda*-cyhalothrin	17%	-	PSD 1988b
		18% [b]	131 days	EU 2001d
1-(2-chlorophenyl)-1-(4'-chlorophenyl)-2,2-dichloroethanol	o,p'-dicofol	43%	30 days	EPA 1998f
2,4'dichlorobenzhydrol	o,p'-dicofol	15%	30 days	EPA 1998f

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Anaerobic soil (laboratory) continued...				
1,1-(p-chlorophenyl)-2,2-dichloroethanol	p,p'-dicofol	major [g]	-	EPA 1998f
4,4'-dichlorobenzhydrol	p,p'-dicofol	major [g]	-	EPA 1998f
4-chlorophenyl urea	diflubenzuron	37% [n]	2 - 14 days	EPA 1997a
2,6-difluorobenzoic acid	diflubenzuron	23% [n]	-	EPA 1997a
decamethrinic acid	deltamethrin	52% [b]	59 days	EU 2002g
		11% [b]	32 days	EU 2002g
ethyl-m-hydroxyphenyl carbamate	desmedipham	28%	-	PSD 1993d
		78% [b]	1 day	EU 2004e
1,3-diphenyl urea	desmedipham	<0.2%	-	PSD 1993d
aniline	desmedipham	69% [b]	1 day	EU 2004e
N-phenyl carbamic acid-ethyl ester	desmedipham	<0.2%	-	PSD 1993d
dimethylaminosulfanilide	dichlofluanid	23.3% [b]	-	HSE 2003a
methylaminosulfanilide	dichlofluanid	0.2% [b]	-	HSE 2003a
diclofop acid	diclofop-methyl	64 - 81%	64 days	PSD 1991c
4-(2,4-dichlorophenoxy)phenol	diclofop-methyl	trace	-	PSD 1991c
N,N-dimethylacetoacetamide	dicrotophos	48%	33 days	EPA 2002b
hydroxyl-N,N-dimethylacetoacetamide	dicrotophos	13%	33 days	EPA 2002b
O-desmethyldimethoate	dimethoate	10%	60 days	PSD 1993f
		10%	14 days	EPA 1999e
O,O-dimethylphosphorothioic acid	dimethoate	5%	60 days	PSD 1993f
		4 - 5%	14 -32 days	EPA 1999e
3-desmethyl dimethomorph and 4-desmethyl dimethomorph combined	dimethomorph	15%	7 days	PSD 1994g
3-desmethyl dimethomorph and 4-desmethyl dimethomorph combined	dimethomorph	~10 - 20%	7 days	PSD 1994g
N'-(3,4-dichlorophenyl)-N-methylurea	diuron	10.3%	45 days	EPA 2003b
EPTC sulfoxide	EPTC	≤0.2%	-	EPA 1999c
$CONH_2$-fen	esfenvalerate	1%	30 days	PSD 1992c
4'-OH-fen	esfenvalerate	4%	30 days	PSD 1992c
Cl-Vacid	esfenvalerate	4%	30 days	PSD 1992c
SD 50365	esfenvalerate	0.4%	30 days	PSD 1992c
IN-JS940	famoxadone	major [g]	-	PMRA 2003h
IN-KZ007	famoxadone	minor [g]	-	PMRA 2003h
IN-H3310	famoxadone	minor [g]	-	PMRA 2003h
RH-9129	fenbuconazole	minor	-	PMRA 2003i
RH-9130	fenbuconazole	minor	-	PMRA 2003i
RH-6467	fenbuconazole	minor	-	PMRA 2003i
aminofenitrothion	fenitrothion	65%	1 week	APVMA 1999
3-methyl-4-nitrophenol	fenitrothion	<10%	-	APVMA 1999
3-phenoxybenzoic acid	fenpropathrin	71%	-	PSD 1989a
2,2,3,3-tetramethyl cyclopropane carboxylic acid	fenpropathrin	39%	8 weeks	PSD 1989a
compound VII	fluazinam	31.2%	90 days	PSD 1994i
		major [g]	-	PMRA 2003j
compound VIII	fluazinam	12%	30 days	PSD 1994i
		major [g]	-	PMRA 2003j
compound XII	fluazinam	7.2%	30 days	PSD 1994i
		major [g]	-	PMRA 2003j
RH-4515	fluoroglycofen-ethyl	10.1%	68 days	PSD 1992d
RH-5781	fluoroglycofen-ethyl	47.7%	2 days	PSD 1992d
RH-5349	fluoroglycofen-ethyl	5%	2 days	PSD 1992d
RH-9985	fluoroglycofen-ethyl	2.7%	2 days	PSD 1992d
RH-4514	fluoroglycofen-ethyl	7.9%	68 days	PSD 1992d
1,2,4-triazole	fluquinconazole	39.7 - 68.1%	399 days	PSD 1999b
FBC 96912	fluquinconazole	53 - 73.8%	399 days	PSD 1999b
4-amino-3,5-dichloro-6-fluoromethoxypyridine	fluroxypyr	12% [b]	112 days	EU 1999
AE F130619	formasulfuron	minor [g]	-	PMRA 2003k
AE F092944	formasulfuron	minor [g]	-	PMRA 2003k
AE F153745	formasulfuron	minor [g]	-	PMRA 2003k
AE F148003	formasulfuron	minor [g]	-	PMRA 2003k
AE F099095	formasulfuron	minor [g]		PMRA 2003k
carbamoylphosphonic acid	foseamine-ammonium	59%	14 days	EPA 1995d
carboxylphosphonic acid	foseamine-ammonium	43%	9 months	EPA 1995d
3-methyl phosphinico-proprionic acid	glufosinate ammonium	54%	26 days	PSD 1990f
		41%	60 days	PSD 1990f
HOE 64619	glufosinate ammonium	22%	26 days	PSD 1990f
M1	imazaquin	0.2%	2 months	PSD 1993h
ioxynil	ioxynil octanoate	12.2% [b]	14 days	EU 2004g
4-hydroxybenzonitrile	ioxynil octanoate	31.5% [b]	28 days	EU 2004g
RP 30228	iprodione	53% [b]	81 days	EU 2002n
N-3,4-dichlorophenyl-N-methylurea	linuron	55% [b]	119 days	EU 2002q
malathion dicarboxylic acid	malathion	26%	62 days	PSD 1995l
malic acid and lactic acid combined	malathion	52%	62 days	PSD 1995l

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Anaerobic soil (laboratory) continued...				
ethylenethiourea	mancozeb	30% [b]	-	EU 2005h
ethyleneurea	mancozeb	12% [b]	-	EU 2005h
CGA-62826	metalaxyl	54.4%	89 days	EPA 1994c
methiocarb phenol	methiocarb	47% [b]	64 days	PSD 1998b
methiocarb sulfoxide	methiocarb	24% [b]	0 days	PSD 1998b
methiocarb sulfoxide phenol	methiocarb	8% [b]	0 days	PSD 1998b
methiocarb sulfone	methiocarb	<1% [b]	64 days	PSD 1998b
methiocarb sulfone phenol	methiocarb	<1% [b]	15 days	PSD 1998b
ethylenethiourea and ethyleneurea combined	metiram	36% [g]	1 day	EU 2005l
metolachlor oxanilic acid	metolachlor	23.33%	29 days	EPA 1995f
CGA-37735	metolachlor	1.25%	29 days	EPA 1995f
CGA-41638	metolachlor	8.3%	60 days	EPA 1995f
CGA-13656	metolachlor	1.46%	29 days	EPA 1995f
CGA-50720	metolachlor	7.34%	60 days	EPA 1995f
S-methyl-N-hydroxythioacetimidate	methomyl	≤3%	-	EPA 1998h
HMUD	nicosulfuron	8.7%	90 days	PSD 2000c
ADMP	nicosulfuron	10.5 - 14.9%	-	PSD 2000c
		4.8% [g]	-	PSD 2000c
		<3.3%	-	PSD 2000c
AUSN	nicosulfuron	10.9 - 19%	-	PSD 2000c
UCSN	nicosulfuron	4.6%	-	PSD 2000c
IN-V9367	nicosulfuron	major [g]	-	PMRA 1996b
IN-J290	nicosulfuron	major [g]	-	PMRA 1996b
2,6-dinitro-3,4-xylidine	pendimethalin	minor [g]	-	EPA 1997d
4-[(1-ethylpropyl)amino]-2-methyl-3,5-dinitro benzyl alcohol	pendimethalin	minor [g]	-	EPA 1997d
4-[(1-ethylpropyl)amino]-3,5-dinitro-o-toluic acid	pendimethalin	minor [g]	-	EPA 1997d
NER	phenmedipham	74.3% [b]	97 days	EU 2004i
MHPC	phenmedipham	19% [b]	32 days	EU 2004i
CL 153815	picolinafen	87% [b]	63 days	PMRA 2003m
dichlorobenzoic acid	piperalin	58%	60 days	EPA 1994e
3-(2-methylpiperi-dino) propyl alcohol	piperalin	14%	60 days	EPA 1994e
CGA-171683	primisulfuron methyl	71.1%	-	PMRA 2001a
saccharin	primisulfuron methyl	32.2%	-	PMRA 2001a
CGA-177288	primisulfuron methyl	5.7%	-	PMRA 2001a
CGA-120844	primisulfuron methyl	9%	-	PMRA 2001a
propachlor alcohol	propachlor	37.3%	9 months	EPA 1998j
Ro 17-3102	propaquizafop	29.4 - 31.6%	-	PSD 1994n
Ro 16-1976	propaquizafop	5.1 - 12.1%	-	PSD 1994n
Ro 40-2724	propaquizafop	5.7 - 12.1%	-	PSD 1994n
2-(3,5-dichlorophenyl)-4,4-dimethyl-5-methyleneoxazoline	propyzamide	17.6%	123 days	EU 2003q
3,5-dichlorobenzoic acid	propyzamide	6.2%	123 days	EU 2003q
CGA 180777	pymetrozine	84.4%	-	PMRA 2002
pymetrozine metabolite III	pymetrozine	20.2%	-	PMRA 2002
pymetrozine metabolite I	pymetrozine	11.5%	-	PMRA 2002
CGA 249257	pymetrozine	13.2%	-	PMRA 2002
GS23199	pymetrozine	15.6%	-	PMRA 2002
CGA 319251	pymetrozine	minor [g]	-	PMRA 2002
CGA 294849	pymetrozine	minor [g]	-	PMRA 2002
CGA 215525	pymetrozine	minor [g]	-	PMRA 2002
CGA 249257	pymetrozine	minor [g]	-	PMRA 2002
CGA 313124	pymetrozine	minor [g]	-	PMRA 2002
BF 500-3	pyraclostrobin	major [g]	-	PMRA 2003n
BF 500-4	pyraclostrobin	major [g]	-	PMRA 2003n
BF 500-5	pyraclostrobin	minor [g]	-	PMRA 2003n
BH518-2	quinmerac	9.9%	63 days	PSD 1998c
BH518-1 and BH518-3 combined	quinmerac	17.3%	31 days	PSD 1998c
IN-70941	rimsulfuron	5.5 - 6.1%	60 days	PSD 1996f
IN-70942	rimsulfuron	46.8 - 55.9%	60 days	PSD 1996f
IN-E9260	rimsulfuron	22.7%	60 days	PSD 1996f
IN-J290	rimsulfuron	6.4%	60 days	PSD 1996f
IN-T5831	rimsulfuron	1%	60 days	PSD 1996f
3,4-dichloro-2,4-difluoroaniline	tebflubenzuron	1%	-	PSD 1991g
3,5-dichloro-2,4-difluorophenyl urea	tebflubenzuron	28.2%	-	PSD 1991g
2,3,5,6-tetrachloroaniline	tecnazene	98.3% [g]	28 days	PSD 1995p
		94.6% [g]	60 days	PSD 1995p
2,3,5,6-tetrachlorothioanisole	tecnazene	3% [g]	60 days	PSD 1995p
2,3,5,6-tetrafluoro-4-methylbenzoic acid	tefluthrin	12% [b]	90 days	PSD 1991h
		13.2% [b]	-	PSD 1991h
2,3,5,6-tetrafluoro-1,4-benzene dicarboxylic acid	tefluthrin	0.2% [b]	90 days	PSD 1991h
		2%	-	PSD 1991h

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Anaerobic soil (laboratory) continued...				
tefluthrin compound V	tefluthrin	<0.1%	7 days	PSD 1991h
PP890	tefluthrin	17%	94 days	PSD 1991h
DP-1	tepraloxydim	12.1%	-	PMRA 2004b
DP-2	tepraloxydim	minor [g]	-	PMRA 2004b
DP-6	tepraloxydim	minor [g]	-	PMRA 2004b
thifensulfuron acid	thifensulfuron-methyl	major [g]	-	EU 2001g
methomyl	thiodicarb	63.4% [b]	3 days	PSD 1992f
methomyl oxime	thiodicarb	21.6 % [b]	7 days	PSD 1992f
TM-CH2OH	tolclofos-methyl	0.7 % [b]	60 days	PSD 1993l
TM-COOH	tolclofos-methyl	0.4 % [b]	60 days	PSD 1993l
TMO	tolclofos-methyl	1.9 % [b]	60 days	PSD 1993l
TMO-CH2OH	tolclofos-methyl	0.7 % [b]	60 days	PSD 1993l
TMO-COOH	tolclofos-methyl	0.2 % [b]	60 days	PSD 1993l
DM-TM	tolclofos-methyl	7.7 % [b]	60 days	PSD 1993l
DM-TMO	tolclofos-methyl	2.5 % [b]	60 days	PSD 1993l
ph-CH3	tolclofos-methyl	3.7 % [b]	60 days	PSD 1993l
ph-CH2OH	tolclofos-methyl	0.3 % [b]	60 days	PSD 1993l
ph-COOH	tolclofos-methyl	0.6 % [b]	60 days	PSD 1993l
tralkoxydim metabolite 9	tralkoxydim	5.4% [c]	3 days	PSD 1993m
tralkoxydim metabolite 8	tralkoxydim	8.3% [b]	3 days	PSD 1993m
tralkoxydim metabolite 10	tralkoxydim	30.9% [b]	61 days	PSD 1993m
CGA 150829	triasulfuron	16.2%	-	PSD 1992g
triazamate metabolite II	triazamate	98% [b]	14 days	PSD 1998d
triazamate metabolite IV	triazamate	20% [b]	-	PSD 1998d
triazamate metabolite IX	triazamate	13% [b]	-	PSD 1998d
triazamate metabolite VIII	triazamate	6% [b]	-	PSD 1998d
SAS 9256	triazoxide	23% [b]	60 days	PSD 1993n
SAS 9709	triazoxide	3% [b]	30 days	PSD 1993n
O-demethyl tribenuron-methyl	tribenuron-methyl	16% [g]	117 days	EFSA 2004
α,α,α-trifluoro-5-nitro-N4,N4-dipropyl-toluene-3,4-diamine	trifluralin	5.4 - 13.2%	60 days	EPA 1996h
7-amino-2-ethyl-1-propyl-5-(trifluoromethyl) benzimidazole	trifluralin	7.3 - 8.3%	60 days	EPA 1996h
α,α,α-trifluoro-N4,N4-dipropyl-toluene-3,4,5-triamine	trifluralin	0.3 - 4.1%	-	EPA 1996h
α,α,α-trifluoro-2,6-dinitro-N-propyl-p-toluidine	trifluralin	≤2.1%	-	EPA 1996h
α,α,α-trifluoro-5-nitro-N4-propyl-toluidine-3,4-diamine	trifluralin	≤2.1%	-	EPA 1996h
2-ethyl-7-nitro-1-propyl-5-(trifluoromethyl) benzimidazole	trifluralin	≤2.1%	-	EPA 1996h
2,2'-azoxybis (α,α,α-trifluoro-6-nitro-N-propyl-p-toluidine	trifluralin	≤2.1%	-	EPA 1996h
2-ethyl-7-nitro-1-propyl-5-(trifluoromethyl) benzimidazole-3-oxide	trifluralin	≤1%	-	EPA 1996h
7-amino-2-ethyl-5-(trifluoromethyl) benzimidazole	trifluralin	≤1%	-	EPA 1996h
methyl saccahrin	triflusulfuron-methyl	74.6% [b]	67 days	PSD 1995r
triazine amine B	triflusulfuron-methyl	56.9% [b]	67 days	PSD 1995r
trinexapac acid	trinexapac-ethyl	major [g]	-	PMRA 2001b
RPA 406341	triticonazole	<2.1%	-	PSD 2000d
		11%	-	PMRA 2000f
RPA 406766	triticonazole	<2.1%	-	PSD 2000d
RPA 405826	triticonazole	<2.1%	-	PSD 2000d
RH-24549	zoxamide	major [g]	-	PMRA 2001d
RH-127450	zoxamide	major [g]	-	PMRA 2001d
Sediment /water systems				
2,4-dichlorophenol	2,4-D	0.5% (estuarine sediment)	33 days	PSD 1993a
2,4-D	2,4-DB	3.5 - 4.6% (sediment)	14 days	EU 2002a
2',6'-diethyl-N-methoxymethyl-2-methyl thioacetanilide	alachlor	2.7%	30 days	PSD 1990a
2',6'-diethyl-N-methoxymethyl acetanilide	alachlor	27.7% (anaerobic)	1 week	PSD 1990a
aldicarb acid	aldicarb	48.6%	50 hours	APVMA 2001
aldicarb nitrile	aldicarb	14.2% (water, anaerobic)	10 days	APVMA 2001
		2.71% (sediment, anaerobic)	14 days	APVMA 2001
aldicarb oxime	aldicarb	~2% (water, anaerobic)	14 days	APVMA 2001
aldicarb alcohol	aldicarb	~2% (water, anaerobic)	14 days	APVMA 2001

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Sediment /water systems continued...				
aldicarb amide	aldicarb	~2% (water, anaerobic)	14 days	APVMA 2001
aldicarb sulfoxide	aldicarb	0.09% (water, anaerobic)	14 days	APVMA 2001
		0.31% (sediment anaerobic)	14 days	APVMA 2001
aldicarb sulfoxide oxime	aldicarb	<1% (sediment anaerobic)	-	APVMA 2001
aldicarb sulfone nitrile	aldicarb	<1% (sediment anaerobic)	-	APVMA 2001
2-amino-4,6-dihydroxypyrimidine	amdosulfuron	45%	84 days	PSD 1994a
HOE 101630	amidosulfuron	30%	61 days	PSD 1994a
BTS 27271	amitraz	primary [g]	-	EPA 1996a
BTS 27919	amitraz	primary [g]	-	EPA 1996a
amitrole metabolite A	amitrole	7% (anaerobic)	39 weeks	EPA 1996b
amitrole metabolite B	amitrole	2% (anaerobic)	26 weeks	EPA 1996b
dihydroxy anilazine	anilazine	8.5% (water)	57 days	PSD 1994b
		0.9% (sediment)	57 days	PSD 1994b
monohydroxy anilazine	anilazine	34.3% (water)	7 days	PSD 1994b
		1.4% (sediment)	1 day	PSD 1994b
monoamino anilazine	anilazine	0.6% (water)	4 days	PSD 1994b
		0.9% (sediment)	4 days	PSD 1994b
sulphanilamide	asulam	2.2% [d]	273 days	EPA 1995a
		3.6% (anaerobic)	366 days	EPA 1995a
asulam metabolite 2	asulam	10.7% (anaerobic)	30 days	EPA 1995a
		7.8% [b]	30 days	EPA 1995a
asulam metabolite 3	asulam	2.9% (anaerobic)	260 days	EPA 1995a
		19.8% [b]	30 days	EPA 1995a
conjugated form of asulam	asulam	23.8% (anaerobic)	1 day	EPA 1995a
		6.1% [b]	273 days	EPA 1995a
acetyl asulam	asulam	14.3% (anaerobic)	7 days	EPA 1995a
deethylatrazine	atrazine	<10% (anaerobic)	-	EPA 2003a
		5.2%	238 days	APVMA 1997a
deisopropylatrazine	atrazine	<10% (anaerobic)	-	EPA 2003a
hydroxyatrazine	atrazine	<10% (anaerobic)	-	EPA 2003a
		16.2% (anaerobic)	238 days	APVMA 1997a
diaminochlorotriazine	atrazine	<10% (anaerobic)	-	EPA 2003a
deethylhydroxyatrazine	atrazine	<10%	-	EPA 2003a
deisopropylhydroxyatrazine	atrazine	<10%	-	EPA 2003a
reference compound 2	azoxystrobin	major [g]	-	PMRA 2000a
reference compound 3	azoxystrobin	minor [g]	-	PMRA 2000a
benalaxyl M1	benalaxyl	7.3% [b] (water)	100 days	EU 2004c
methyl-N-phenylacetyl-N-(2-carboxy-6-methyl)phenyl DL-alinate	benalaxyl	1.38% [b] (sediment)	100 days	EU 2004c
benalaxyl acid	benalaxyl	5.38% [b] (sediment)	100 days	EU 2004c
N-methylbentazone	bentazone	7.2 - 12.5% [b] (water)	30 days	EU 2000a
bitertanol ketone	bitertanol	< 1%	120 days	PSD 1994c
bitertanol benzoic acid	bitertanol	< 1%	120 days	PSD 1994c
3-sec-butyl-6-methyluracil	bromacil	80.7% [b]	304 days	EPA 1996c
3,5-dibromo-4-hydroxy-benazmide	bromoxynil	23.3% [b] (water)	14 days	EU 2004d
		3.2% [b] (sediment)	14 days	EU 2004d
bromoxynil	bromoxynil octanoate	40.1% [b] (water)	7 days	EU 2004d
		8.5% [b] (sediment)	7 days	EU 2004d
		63.1% b (water)	2 days	EU 2004d
		<2.1% (sediment)	-	EU 2004d
4-hydroxy benzonitrile	bromoxynil octanoate	36.1% [b] (water)	14 days	EU 2004d
		9.4% [b] (sediment)	14 days	EU 2004d
		16.3% [b] (water)	14 days	EU 2004d
		9.3% [b] (soil)	14 days	EU 2004d
		25.4% [b] (water)	30 days	EU 2004d

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Sediment /water systems continued...				
		<7.5% (sediment)	30 days	EU 2004d
		45.52% [b] (anaerobic)	14 days	EPA 1998c
3,5-dibromo-4-hydroxybenzonitrile	bromoxynil octanoate	66.1% [b] (water)	2 days	EU 2004d
		41.5% [b] (soil)	0.5 days	EU 2004d
		48.5% [b] (anaerobic)	7 days	EPA 1998c
		78.77% [b]	2 days	EPA 1998c
3,5-dibromo-4-hydroxybenzoic acid	bromoxynil octanoate	11.3% [b] (water)	21 days	EU 2004d
		5% b (soil)	30 days	EU 2004d
3-bromo-4-hydroxybenzonitrile	bromoxynil octanoate	12.1% [b] (water)	7 days	EU 2004d
		11.5% [b] (water)	7 days	EU 2004d
		1% [b] (sediment)	7 days	EU 2004d
LS 860550	bromuconazole	<1% (water)	-	PSD 1996a
LS 860364	bromuconazole	<1% (water)	-	PSD 1996a
LS 830730	bromuconazole	<1% (water)	-	PSD 1996a
buprofezin sulphoxide	buprofezin	13%	56 days	PSD 1993b
tetrahydrophthalamide	captan	81.2%	0 days	EPA 1999a
		51.1%	30 days	EPA 1999a
THPAm	captan	27%	7 days	EPA 1999a
THPAI	captan	10.8%	14 days	EPA 1999a
THPI epoxide	captan	9.4%	1 days	EPA 1999a
2,4-dichloro-1-(1-hydroxyethyl) benzene	chlorfenvinphos	11.2% [b] (sediment)	63 days	APVMA 2000a
		27.7% [b] (water)	63 days	APVMA 2000a
		10.6 - 17.4% [b] (sediment)	61 days	APVMA 2000a
5-cyano-4,6,7-tichloro2H-1,2-benzisothiazol-3-one	chlorothalonil	30.9% (fresh water)	1 day	PSD 2002
		29.2% (saltwater)	30 days	PSD 2002
		25 - 30%	-	EPA 1999b
SDS-67042 sulphoxide	chlorothalonil	16.5% (fresh water)	9 days	PSD 2002
		12.1% (saltwater)	9 days	PSD 2002
		15%	-	EPA 1999b
2,5,6-trichloro-4-(glutathione-5-yl)isophthalonitrile	chlorothalonil	<10% (fresh water)	-	PSD 2002
		<10% (saltwater)	-	PSD 2002
2,5,6-trichloro-4-(thio)isophthalonitrile	chlorothalonil	<10% (fresh water)	-	PSD 2002
		<10% (saltwater)	-	PSD 2002
4-hydroxy-2,5,6-trichloroisophthalonitrile	chlorothalonil	5.4% (fresh water)	-	PSD 2002
		30 - 40% (anaerobic)	1 - 2 months	EPA 1999b
		5 - 10%	-	EPA 1999b
two isomers of 3-cyano-2,5,6-trichlorobenzamide combined	chlorothalonil	9% (anaerobic)	-	EPA 1999b
3-cyano-2,4,5,6-tetrachlorobenzamide	chlorothalonil	7% (anaerobic)	-	EPA 1999b
3-cyano-6-hydroxy-2,4,5-trichlorobenzamide	chlorothalonil	4% (anaerobic)	-	EPA 1999b
3-carbamyl-1,2,4,5-trichlorobenzoic acid	chlorothalonil	≤3% (anaerobic)	-	EPA 1999b
3-(3-chloro-p-tolyl)-1-methylurea	chlorotoluron	12.6% (water)	49 days	EU 2005c
chlorotoluron benzoic acid	chlorotoluron	25.1% (water)	100 days	EU 2005c
3-chloroaniline	chlopropham	9.9% [b] (sediment)	42 days	EU 2003b
3,5,6-trichloro-2-pyrindinol	chlorpyrifos-methyl	20 - 35% (sediment)	30 days	EU 2005e
		37 - 60% (water)	30 days	EU 2005e
clodinafop acid	clodinafop-propargyl	~100% (anaerobic)	28 days	PSD 1995a
		97.6% [b]	4 days	PSD 1995a
CGA 302371	clodinafop-propargyl	10.5% (anaerobic)	245 days	PSD 1995a
		45.9%	119 days	PSD 1995a
CCIM	cyazofamid	20.8 - 29% [g] (water)	21 - 30 days	EU 2002e
		13.3 - 19.5% (sediment)	21 - 30 days	EU 2002e
CCIM-AM	cyazofamid	4% [g] (water)	-	EU 2002e

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Sediment /water systems continued...				
		7.2% [g] (sediment)	-	EU 2002e
CTCA	cyazofamid	8.8% [g] (water)	100 days	EU 2002e
		16.2 - 24.6% [g] (sediment)	100 days	EU 2002e
TSO and T2SO combined	cycloxydim	19 - 82% (pH 9.4)	28 days	PSD 1990b
4-fluoro-3-phenoxybenzaldehyde	cyfluthrin	1.1% [b] (water)	1 day	EU 2002c
		16% [b] (sediment)	1 day	EU 2002c
4-fluoro-3-phenoxybenzoic acid	cyfluthrin	29% [b] (water)	11 days	EU 2002c
		24% [b] (sediment)	1 day	EU 2002c
DCVA	cyfluthrin	32.2 - 36% [b] (water)	28 days	EU 2002c
		11.2 - 25.6% [b] (sediment)	100 days	EU 2002c
compound Ia	cyhalothrin and *lambda*-cyhalothrin	26.9 - 32%	32 days	PSD 1988b
		11% [b] (water)	30 days	EU 2001d
		11% [b] (sediment)	30 days	EU 2001d
compound Ib	cyhalothrin	9 - 15.3%	32 days	PSD 1988b
compound XV	*lambda*-cyhalothrin	<10%	-	EU 2001d
3-phenoxybenzoic acid	*lambda*-cyhalothrin	<10%	-	EU 2001d
3-phenoxybenzylalcohol	*lambda*-cyhalothrin	<10%	-	EU 2001d
aminooxacetic acid	cymoxanil	minor [g]	-	PMRA 2000b
JX915	cymoxanil	minor [g] (anaerobic)	-	PMRA 2000b
W3595	cymoxanil	minor [g] (anaerobic)	-	PMRA 2000b
U3204	cymoxanil	minor [g]	-	PMRA 2000b
T4226	cymoxanil	minor [g]	-	PMRA 2000b
KP533	cymoxanil	minor [g] (anaerobic)	-	PMRA 2000b
R3273	cymoxanil	minor [g]	-	PMRA 2000b
3-phenoxybenzoic acid	*alpha*-cypermethrin	23% [b]	7 days	EU 2004b
dimethylcyclopropane carboxylic acid	*alpha*-cypermethrin	47% [b] (water)	14 days	EU 2004b
		19.5% [b] (sediment)	14 days	EU 2004b
CGA 249287	cyprodinil	14% [b] (sediment)	112 days	EU 2004b
formaldehyde	daminozide	17% [g] (sediment)	7 days	EU 2005g
		9.5% [g] (water)	7 days	EU 2005g
α-R-deltamethrin	deltamethrin	21 - 24% [b]	1 - 2 weeks	EU 2002g
ethyl-m-hydroxyphenyl carbamate	desmedipham	84% (water)	7 days	PSD 1993d
		1.7% (sediment)	21 days	PSD 1993d
		96% [b] (water)	1 day	EU 2004e
		13% [b] (sediment)	100 days	EU 2004e
		87.7% (anaerobic)	15 days	EPA 1996e
aniline	desmedipham	72% [b] (water)	0 days	EU 2004e
diclofop acid	diclofop-methyl	70%	7 days	PSD 1991c
		40.2% (water)	14 days	PSD 1991c
		77.9 % (sediment)	168 days	PSD 1991c
4-(2,4-dichlorophenoxy)phenol	diclofop-methyl	10%	7 days	PSD 1991c
		52.4 % (sediment)	168 days	PSD 1991c
N'-(3-chlorophenyl)-N,N-dimethylurea	diuron	25% (whole system)	-	EPA 2003b
		major [g] (anaerobic)	-	EPA 2003b
N'-(3,4-dichlorophenyl)-N-methylurea	diuron	minor [g] (sediment)	-	EPA 2003b
3-chlorophenyl methylurea	diruon	minor [g] (sediment)	-	EPA 2003b
phenyl-1,1-dimethylurea	diuron	minor [g] (anaerobic)	-	EPA 2003b
N'-(3-chlorophenyl)-N-methyl urea	diuron	minor [g] (anaerobic)	-	EPA 2003b
210 352	epoxiconazole	0.4 - 1.1%	90 days	PSD 1994h
231 761	epoxiconazole	0.4 - 0.9%	90 days	PSD 1994h
CIPA	esfenvalerate	44 -48%	100 days	EU 2000b

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Sediment /water systems continued...				
3-phenoxybenzoic acid	esfenvalerate	2 - 13%	30 days	EU 2000b
triazine amine C	ethametsulfuron-methyl	major	-	PMRA 1992
saccharin	ethametsulfuron-methyl	major	-	PMRA 1992
ethametsulfuron-methyl acid	ethametsulfuron-methyl	major	-	PMRA 1992
ethylene	ethephon	50.6 - 52.1% (anaerobic)	14 days	EPA 1995b
2-hydroxy ethyl phosphonic acid	ethephon	42.6% (anaerobic)	30 days	EPA 1995b
IN-JS940	famoxadone	major [g] (water)	-	PMRA 2003h
IN-H3310	famoxadone	major [g] (sediment)	-	PMRA 2003h
IN-KZ007	famoxadone	minor [g]	-	PMRA 2003h
IN-JL856	famoxadone	minor [g]	-	PMRA 2003h
WAK 6920	fenhexamid	<10% (anaerobic)	-	PMRA 2003b
KBR 6720	fenhexamid	<10% (anaerobic)	-	PMRA 2003b
KBR 7133	fenhexamid	<10% (anaerobic)	-	PMRA 2003b
KBR 7115	fenhexamid	<10% (anaerobic)	-	PMRA 2003b
N-acetyl-2,3-dichloro-p-aminophenol	fenhexamid	<10% (anaerobic)	-	PMRA 2003b
3-methyl-4-nitrophenol	fenitrothion	major [g]	-	PMRA 1993a
		major [g] (anaerobic)	-	PMRA 1993a
		15% (anaerobic)	2 days	APVMA 1999
aminofenitrothion	fenitrothion	major [g]	-	PMRA 1993a
		13% (anaerobic)	3 days	APVMA 1999
acetlaminofenitrothion	fenitrothion	13% (anaerobic)	3 days	APVMA 1999
formylaminofenitrothion	fenitrothion	5% (anaerobic)	7 days	APVMA 1999
desmethyl fenitrothion	fenitrothion	<1.5% (anaerobic)	-	APVMA 1999
desmethyl fenitrooxon	fenitrothion	<1.5% (anaerobic)	-	APVMA 1999
3-methyl-4-nitroanisole	fenitrothion	<1.5% (anaerobic)	-	APVMA 1999
fenoxaprop-ethyl acid	fenoxaprop-ethyl	47% (water)	1 day	PSD 1990c
6-chloro-3-dihydrobezoxazol-2-one	fenoxaprop-ethyl	9.3% (water)	21 days	PSD 1990c
fenoxaprop-ethyl acid	fenoxaprop-ethyl	60.4% (sediment)	29 days	PSD 1990c
6-chloro-3-dihydrobezoxazol-2-one	fenoxaprop-ethyl	3.8% (sediment)	21 days	PSD 1990c
R0 15-6045	fenpropidin	15 - 16 %	28 - 84 days	PSD 1993g
M3	fenpyroximate	5.8 - 18.3% [d] (water)	24 hours	PSD 1995d
		4.6 - 16.1%	90 days	PSD 1995d
1,3-dimethyl-5-phenoxypyrazole-4-carbonitrile	fenpyroximate	<5% [d] (water)	24 hours	PSD 1995d
MB 45950	fipronil	<8.8% (water)	-	PSD 2004a
		~80% (sediment)	-	PSD 2004a
RPA 200766	fipronil	<8.8% (water)	-	PSD 2004a
		<6.6% (sediment)	-	PSD 2004a
MB 46126	fipronil	<8.8% (water)	-	PSD 2004a
		<6.6% (sediment)	-	PSD 2004a
5-hydroxy-XDE-570	florasulam	major [g]	-	PMRA 2001c
		87%[b] (anaerobic)	97 days	PMRA 2001c
N-(2,6-difluorophenyl-5-aminosulphonyl-1H-1,2,4-triazole-3-carboxylic acid	florasulam	major [g]		PMRA 2001c
triazolosulfonic carboxylic acid	florasulam	major [g]		PMRA 2001c
compound XII	fluazinam	8%	0 weeks	PSD 1994i
DCPA	fluazinam	major [g]	-	PMRA 2003j
compound V	fluazinam	major [g]	-	PMRA 2003j
compound VIII	fluazinam	major [g]	-	PMRA 2003j
		19% (anaerobic)	30 days	PMRA 2003j
AMPA	fluazinam	major [g]	-	PMRA 2003j
		major [g] (anaerobic)	-	PMRA 2003j
SDS-67200	fluazinam	major [g] (anaerobic)	-	PMRA 2003j
MKH 6562 sulfonamide	flubcarbazone-sodium	14.9 - 16.1%	-	PMRA 2000c
		89% (anaerobic)		PMRA 2000c
MKH 6562 sulfonic acid	flubcarbazone-sodium	<0.8%	-	PMRA 2000c

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Sediment /water systems continued...				
NODT	flubcarbazone-sodium	19%	-	PMRA 2000c
		3.7 - 7% (anaerobic)	-	PMRA 2000c
NMT	flubcarbazone-sodium	65% (anaerobic)	-	PMRA 2000c
FOE alcohol	flufenacet	minor [g]	365 days	PMRA 2000d
FOE oxalte	flufenacet	24%	365 days	PMRA 2000d
FOE sulfonic acid	flufenacet	minor [g]	365 days	PMRA 2000d
FOE amine acetate	flufenacet	minor [g] (anaerobic)	-	PMRA 2000d
thiadone	flufenacet	minor [g] (anaerobic)	-	PMRA 2000d
thiadone acetate	flufenacet	minor [g] (anaerobic)	-	PMRA 2000d
1,2,4-triazole	fluquinconazole	16.1%	365 days	PSD 1999b
FBC 96912	fluquinconazole	23.9% (water)	28 days	PSD 1999b
		47% (sediment)	100 days	PSD 1999b
		21.8% (water)	14 days	PSD 1999b
		44.3% (sediment)	100 days	PSD 1999b
SN 616368	fluquinconazole	2.1% (water)	-	PSD 1999b
4-amino-3,5-dichloro-6-fluoro-2-pyridinol	fluroxypyr	44% [b] (water)	14 days	EU 1999
		13.2% [b] (sediment)	7 days	EU 1999
4-amino-3-chloro-6-fluoro-2-pyridinol	fluroxypyr	17.9% [b] (water)	28 days	EU 1999
		6.5% [b] (sediment)	28 days	EU 1999
4-amino-3,5-dichloro-6-fluoro-2-pyridone	fluroxypyr	45% [b] (whole system)	8 weeks	EU 1999
RE 53285	flurtamone	<4%	-	PSD 2000a
		1.2% (anaerobic)		PSD 2000a
RE 54589	flurtamone	<4%	-	PSD 2000a
		0.2% (anaerobic)		PSD 2000a
RE 54488	flurtamone	<4%	-	PSD 2000a
		0.4% (anaerobic)		PSD 2000a
bis (4-fluorophenyl)methyl silanol	flusilazole	48 - 60%	52 weeks	PSD 1989b
1H-1,2,4-triazole	flusilazole	12%	52 weeks	PSD 1989b
AE 0338795	formasulfuron	major [g]	-	PMRA 2003k
		major [g] (anaerobic)	-	PMRA 2003k
AE F153745	formasulfuron	major [g]	-	PMRA 2003k
		minor [g] (anaerobic)	-	PMRA 2003k
AE F130619	formasulfuron	minor [g]	-	PMRA 2003k
		minor [g] (anaerobic)	-	PMRA 2003k
AE F092944	formasulfuron	minor [g]	-	PMRA 2003k
		minor [g] (anaerobic)	-	PMRA 2003k
AE F148003	formasulfuron	minor [g]		PMRA 2003k
		minor [g] (anaerobic)	-	PMRA 2003k
AE F159255	formasulfuron	minor [g]		PMRA 2003k
AE 0014940	formasulfuron	minor [g]		PMRA 2003k
AE F099095	formasulfuron	minor [g] (anaerobic)	-	PMRA 2003k
carbamoylphosphonic acid	foseamine-ammonium	59%	14 days	EPA 1995d
carboxylphosphonic acid	foseamine-ammonium	43%	9 months	EPA 1995d
aminomethylphosphonic acid	glyphosate	16% [b] (water)	14 days	EU 2002l
		major [g] (aerobic)	-	EPA 1993b
		major [g] (anaerobic)	-	EPA 1993b
aminomethylphosphonic acid	glyphosate trimesium	4% [b] (water)	-	EU 2002l
		18% [b] (sediment)	-	EU 2002l
3-hydroxy-cyclohexyl-6-(dimethylamino)-1-methyl-1,3,5-triazine-2,4(1H,-3H)-dione	hexazinone	5.5% (anaerobic, sediment)	365 days	EPA 1994a
3-(ketocyclohexyl)-6-(dimethylamino)-1-methyl-1,3,5-triazine-2,4(1H,3H)-dione	hexazinone	25% (anaerobic, sediment)	365 days	EPA 1994a
3-cyclohexyl-1-methyl-1,3,5-triazine-2,4,6-1H,3H,5H)-trione	hexazinone	24% (anerobic, sediment)	-	EPA 1994a

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Sediment /water systems continued...				
		1.3%	-	EPA 1994a
[3-(4-ketocyclohexyl)-6-(dimethylamino)-1-methyl-1,3,5-triazine-2,4(1H,3H)-dione	hexazinone	<7%	-	EPA 1994a
3-(2-hydroxycyclohexyl)-6-(dimethylamino-1-methyl-1,3,5-triazine-2,4(1H,3H)-dione	hexazinone	<7%	-	EPA 1994a
3-(cyclohexyl-6-(methylamino)-1-methyl-1,3,5-triazine-2,4(1H,3H)-dione]	hexazinone	<7%	-	EPA 1994a
1-(6-chloro-pyridine-3-ylmethyl)-2-imino-imidazolidine	imidacloprid	8.8 - 12.3%		PSD 1993i
		64% (anaerobic)	358 days	PSD 1993i
6-chloro-nicotinic acid	imidacloprid	0.3 - 4.2%		PSD 1993i
N-1-(6-chloro-pyridine-3-ylmethyl)-ethane-1,2-diamine	imidacloprid	0.3 - 4.2%		PSD 1993i
metsulfuron-methyl	iodosulfuron-methyl	major [g]	-	PMRA 2004f
		major [g] (anaerobic)	-	PMRA 2004f
AE F059411	iodosulfuron-methyl	major [g]	-	PMRA 2004f
		minor [g] (anaerobic)	-	PMRA 2004f
AE 0000119	iodosulfuron-methyl	major [g]	-	PMRA 2004f
AE 0014966	iodosulfuron-methyl	major [g]	-	PMRA 2004f
		minor [g] (anaerobic)	-	PMRA 2004f
AE 0034855	iodosulfuron-methyl	major [g]	-	PMRA 2004f
AE 0014965	iodosulfuron-methyl	minor [g]	-	PMRA 2004f
AE F145740	iodosulfuron-methyl	minor [g]	-	PMRA 2004f
		minor [g] (anaerobic)	-	PMRA 2004f
AE F161778	iodosulfuron-methyl	minor [g]	-	PMRA 2004f
		minor [g] (anaerobic)	-	PMRA 2004f
AE F145741	iodosulfuron-methyl	minor [g] (anaerobic)	-	PMRA 2004f
3,5-di-iodo-4-hydroxybenzamide	ioxynil	11.3% [b] (water)	7 days	EU 2004g
		3.6% [b] (sediment)	7 days	EU 2004g
ioxynil	ioxynil octanoate	52.2% [b] (water)	2 days	EU 2004g
		11.8% [b] (sediment)	7 days	EU 2004g
propargyl butyl carbamate	IPBC	>97% (water, anaerobic)	1 day	HSE 1994
		>80% (sterile)	29 days	HSE 1994
2-propenyl butyl-carbamate	IPBC	8% (sediment, anaerobic)	59 days	HSE 1994
2-propenyl butyl-carbamate	IPBC	34.7% (water, anaerobic)	59 days	HSE 1994
RP 35606	iprodione	71.3% (water)	-	EU 2002n
		< 5% (sediment)	-	EU 2002n
RP 30228	iprodione	<10% (water)	24 hours	EU 2002n
		70% (sediment)	-	EU 2002n
		64.6% [b]	14 days	EPA 1998g
		70.7% (anaerobic)	14 days	EPA 1998g
RP 32490	iprodione	14.6% [b]	2 days	EPA 1998g
		8.4% (anaerobic)	30 days	EPA 1998g
3,5-dichloroaniline	iprodione	9.9% [b] (sediment)	30 days	EPA 1998g
desmethylisoptoturon	isoproturon	19.2% [b] (water)	60 days	EU 2002p
		6.8% [b] (sediment)	60 days	EU 2002p
RPA 202248	isoxaflutole	60 - 63%	2 days	PMRA 2000e
		80% (anaerobic)	14 days	PMRA 2000e
		69% (water, anaerobic)	6 hours	PMRA 2000e
		57% (sediment, anaerobic)	183 days	PMRA 2000e
RPA 205834	isoxaflutole	28% (anaerobic)	6 hours	PMRA 2000e
		25% (water, anaerobic)	6 hours	PMRA 2000e
		3% (sediment, anaerobic)	6 hours	PMRA 2000e

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Sediment /water systems continued...				
RPA 203328	isoxaflutole	<1.5% (anaerobic)	-	PMRA 2000e
RPA 207048	isoxaflutole	<1.5% (anaerobic)	-	PMRA 2000e
kresoxim-methyl acid	kresoxim-methyl	7.4%	-	PSD 1997c
3-(3,4-dichlorophenyl)-1-methylurea	linuron	10% (water)	-	PSD 1995h
		2% (sediment)	-	PSD 1995h
3,4-dichlorophenylurea	linuron	1.5% (water)	-	PSD 1995h
		0.5% (sediment)	-	PSD 1995h
malathion monocarboxylic acids	malathion	28% (anaerobic, water)	4 days	PSD 1995i
		4.5% (anaerobic, sediment)	0.25 days	PSD 1995i
malathion dicarboxylic acid	malathion	21% (anaerobic, water)	14 days	PSD 1995i
		5.2% (anaerobic, sediment)	4 days)	PSD 1995i
malathion demethyl dicarboxylic acid	malathion	39% (anaerobic, water)	45 days	PSD 1995i
malathion demethyl monocarboxylic acids	malathion	21% (anaerobic, water)	7 days	PSD 1995i
		8.1% (anaerobic, sediment)	45 days	PSD 1995i
ethylenethiourea	mancozeb	41.9% (river water)	6 hours	PSD 2004b
		48.5% (pond water	1 day	PSD 2004b
		6.3% (river sediment)	2 days	PSD 2004b
		6.6% (pond sediment)	14 days	PSD 2004b
		48.5% [b] (water)	1 day	EU 2005h
		8.1% [b] (sediment)	7 days	EU 2005h
ethyleneurea	mancozeb	37.5% [b] (water)	14 days	EU 2005h
		9.1% [b] (sediment)	30 days	EU 2005h
		22.5% (river water)	30 days	PSD 2004b
		23.4% (pond water	59 days	PSD 2004b
		7.8% (river sediment)	30 days	PSD 2004b
		9.1% (pond sediment)	30 days	PSD 2004b
ethylenebisisothiocyanide sulfide	mancozeb	30.9% [b] (water)	0 days	EU 2005h
		3.8% [b] (sediment)	2 days	EU 2005h
DIDT	mancozeb	12.7% (river water)	6 hours	PSD 2004b
		3.8% (pond water	6 hours	PSD 2004b
		3.8% (river sediment)	2 days	PSD 2004b
		1.1% (pond sediment)	2 days	PSD 2004b
hydantoin	mancozeb	8.6% (river water)	14 days	PSD 2004b
		5.7% (pond water	14 days	PSD 2004b
		3% (river sediment)	14 days	PSD 2004b
		2.2% (pond sediment)	14 days	PSD 2004b
ethylenethiourea	maneb	31.9% [g] (river water)	1 day	EU 2005l
		7% [g] (river sediment)	7 days	EU 2005l
		47.9% [g] (pond water)	2 days	EU 2005l
		13.7% [g] (pond sediment)	7 days	EU 2005l
ethyleneurea	maneb	20.6% [g] (river water)	14 days	EU 2005l
		5.1% [g] (river sediment)	14 days	EU 2005l

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Sediment /water systems continued...				
		23.4% [g] (pond water)	30 days	EU 2005i
		7.3% [g] (pond sediment)	30 days	EU 2005i
ethylenebisisothiocyanide sulfide	maneb	45.5% [g] (river water)	0 days	EU 2005i
		2.6% [g] (river sediment)	7 days	EU 2005i
		41.5% [g] (pond water)	0 days	EU 2005i
		0.7% [g] (pond sediment)	7 days	EU 2005i
HOE 113225	mefenpyr-diethyl	10.4 - 34.3% (sediment)	-	PSD 1999a
		53.5 - 87.9% (water)	-	PSD 1999a
HOE 094270	mefenpyr-diethyl	1.2 - 33.9% (sediment)	-	PSD 1999a
		27.1 - 28.5% (water)	-	PSD 1999a
HOE 109453	mefenpyr-diethyl	4.5 - 5.6% (sediment)	-	PSD 1999a
		38.9 - 42% (water)	-	PSD 1999a
CGA-62826	metalaxyl	85.5% (anaerobic)	265 days	EPA 1994c
		20.56%	30 days	EPA 1994c
CGA-119857	metalaxyl	16.3% (anaerobic)	385 days	EPA 1994c
M13	metconazole	9% [b] (water)	152 days	PSD 2000b
M11, M13, M15, M21, M30 and M119 combined	metconazole	16% [b] (water)	152 days	PSD 2000b
		13% [b] (sediment)	152 days	PSD 2000b
M11, M13, M21, M30 and M119 combined	metconazole	0.5% (water)	-	PSD 2000b
		9% b (sediment)	182 days	PSD 2000b
M30	metconazole	5% [b] (sediment)	152 days	PSD 2000b
M21 and M119 combined	metconazole	5% [b] (sediment)	152 days	PSD 2000b
methiocarb phenol	methiocarb	83% [b] (water)	7 days	PSD 1998b
		45% [b] (anaerobic, water)	3 days	PSD 1998b
		51% [b] (anaerobic, sediment)	28 days	PSD 1998b
methiocarb sulfoxide	methiocarb	1% [b] (water)	0 days	PSD 1998b
		1% [b] (anaerobic, water)	0 days	PSD 1998b
methiocarb sulfoxide phenol	methiocarb	63% [b] (water)	14 days	PSD 1998b
RH-117236	methoxyfenozide	12.6%	91 days	PMRA 2004g
RH-131154	methoxyfenozide	2% (anaerobic)	91 days	PMRA 2004g
ethylenetiourea	metiram	41 - 49% [g]	0.25 days	EU 2005l
		6.4 - 7.6% [g]	7 days	EU 2005l
CGA-41507	metolachlor	3.34% (sediment)	29 days	EPA 1995f
		1.21 (water)	29 days	EPA 1995f
		4.85% (anaerobic, water)	6 months	EPA 1995f
		15.88% (anaerobic, sediment)	12 months	EPA 1995f
CGA-50720	metolachlor	1.17% (sediment)	-	EPA 1995f
		1.67% (anaerobic, sediment)	29 days	EPA 1995f
CGA-40172	metolachlor	1.13% (sediment)	-	EPA 1995f
		5.64% (anaerobic, water)	12 months	EPA 1995f
		3.18% (anaerobic, sediment)	12 months	EPA 1995f
CGA-46127	metolachlor	1.54 (sediment)	-	EPA 1995f

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Sediment /water systems continued...				
		4.69% (anaerobic, water)	12 months	EPA 1995f
		13.02% (anaerobic, sediment)	12 months	EPA 1995f
metolachlor oxanilic acid	metolachlor	1.99% (water)	29 days	EPA 1995f
CGA-37913	metolachlor	4.28% (anaerobic, water)	6 months	EPA 1995f
		2.33% (anaerobic sediment)	6 months	EPA 1995f
acetonitrile	methomyl	46%	102 days	EPA 1998h
acetamide	methomyl	14%	7 days	EPA 1998h
ATSA	metosulam	2.5 - 8.1% (water)	28 days	PSD 1996c
		8.2% (water)	42 days	PSD 1996c
		8.4% (sediment)	42 days	PSD 1996c
dihydroxymetosulam	metosulam	<4%	42 days	PSD 1996c
N-succinyl ATSA	metosulam	<4%	42 days	PSD 1996c
N-acetyl ATSA	metosulam	<4%	42 days	PSD 1996c
saccharin	metsulfuron-methyl	8%	14 days	PSD 1991e
		26 - 33% (sterile)	24 weeks	PSD 1991e
2-(aminosulfonyl) benzoic acid	metsulfuron-methyl	14%	14 days	PSD 1991e
		40% (sterile, anaerobic)	5 weeks	PSD 1991e
		6 - 13% (non-sterile)	-	PSD 1991e
O-desmethyl metsulfuron methyl	metsulfuron-methyl	25% [b] (water)	13 weeks	EU 2000c
		8% [b] (sediment)	8 - 13 weeks	EU 2000c
O-desmethyl metsulfuron methyl acid	metsulfuron-methyl	15 - 31% [b]	13 weeks	PSD 1995n
HMUD	nicosulfuron	17% [g]	-	PSD 2000c
		19% [g]	-	PSD 2000c
AUSN	nicosulfuron	11% [g]	-	PSD 2000c
		7% [g]	-	PSD 2000c
UCSN	nicosulfuron	7%	-	PSD 2000c
		4% [g]	-	PSD 2000c
ASDM	nicosulfuron	9% [g]	-	PSD 2000c
		8% [g]	-	PSD 2000c
desmethyl norflurazon	norflurazon	19% (anaerobic)	365 days	EPA 1996f
		11%	90 days	EPA 1996f
2,2-dithiobis (N-methylacetamide)	omethoate	ND - 8.2%	-	PSD 1993j
N-methyl-2-methylsulfinyl-acetamide	omethoate	ND - 4%	-	PSD 1993j
2-hydroxy-N-methylacetamide	omethoate	ND - 5.7%	-	PSD 1993j
O-methyl-S-2-(methylamino)-2-oxoethylphosphorothioate	omethoate	ND - 27.1	-	PSD 1993j
ketone metabolite	paclobutrazol	<5% (whole system)	-	PSD 1995j
ketol metabolite	paclobutrazol	<5% (whole system)	-	PSD 1995j
diol metabolite	paclobutrazol	<5% (whole system)	-	PSD 1995j
1,2,4-triazole	paclobutrazol	9.4%	12 weeks	PSD 1995j
formaldehyde	phorate	17%	14 days	PMRA 2003a
5,6-dimethyl-2-methylformamido-pyrimidin-4-yl-dimethyl carbamate	pirimicarb	5%		PSD 1994m
5,6-dimethyl-2-methylamino-pyrimidin-4-yl-dimethylcarbamate	pirimicarb	6.4%	-	PSD 1994m
5,6-dimethyl-2-dimethylamino-pyrimidin-4-ol	pirimicarb	3.5%	-	PSD 1994m
CGA-191429	primisulfuron methyl	32 - 44% (river water)	-	PMRA 2001a
		52.4 - 54.1% (pond water)	-	PMRA 2001a
CGA-239771	primisulfuron methyl	25.2% (river water)	-	PMRA 2001a
		16.5% (pond water)	-	PMRA 2001a
		33% (river sediment)	-	PMRA 2001a
		37.1% (pond sediment)	-	PMRA 2001a
CGA-171683	primisulfuron methyl	3.9% (river water)	-	PMRA 2001a

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Sediment /water systems continued...				
		4.8% (pond water)	-	PMRA 2001a
		2.3% (river sediment)	-	PMRA 2001a
		1.8% (pond sediment)		PMRA 2001a
CGA-147087	primisulfuron methyl	2.4% (river water)	-	PMRA 2001a
		4% (pond water)	-	PMRA 2001a
		2.3% (river sediment)	-	PMRA 2001a
		2.6% (pond sediment)	-	PMRA 2001a
CGA-177288	primisulfuron methyl	2.2% (river water)	-	PMRA 2001a
		9.2% (pond water)	-	PMRA 2001a
		1.2% (river sediment)	-	PMRA 2001a
		3.1% (pond sediment)	-	PMRA 2001a
CGA-219741	primisulfuron methyl	4% (river water)	-	PMRA 2001a
		0.9% (pond water)	-	PMRA 2001a
CGA-120844	primisulfuron methyl	0.8% (river sediment)	-	PMRA 2001a
		1% (pond sediment)		PMRA 2001a
CGA-191429	primisulfuron methyl	13.4 - 17% (pond sediment)	-	PMRA 2001a
Ro 16-1976	propaquizafop	1.3 - 14.5% (water)	-	PSD 1994n
		2.3 - 3.2% (sediment)	-	PSD 1994n
Ro 19-5081	propaquizafop	13.3 - 13.8%(water)	-	PSD 1994n
		3.7 - 10.2% (sediment)	-	PSD 1994n
Ro 16-1981	propaquizafop	1% (sediment)	-	PSD 1994n
Ro 16-1981-methyl	propaquizafop	5.3 -9% (sediment)	-	PSD 1994n
	propaquizafop	major [g] (pH 7 and 9)	14 days	PSD 1994n
	propaquizafop	major [g] (pH 5)	14 days	PSD 1994n
CGA 217 495	propiconazole	2.8 - 2.9%	90 - 175 days	EU 2003n
CGA 91305	propiconazole	3.1 - 5.0%	90 - 175 days	EU 2003n
propiconazole M3	propiconazole	3.1 - 4.4%	90 - 175 days	EU 2003n
1,2,4-triazole	propiconazole	2.1 - 2.3%	90 - 175 days	EU 2003n
		5.2% (water)	84 days	PSD 1993g
propylenethiourea	propineb	93.9% [b] (water)	1 hour	EU 2003o
		56.8 % [b] (sediment)	60 days	EU 2003o
6-chloro-3-phenyl-pyridazin-4-ol	pyridate	48 - 58% [b] (water)	1 - 7 days	EU 2001e
		46.7% [b] (sediment)	30 days	EU 2001e
CL 9673-O-methyl	pyridate	9 - 12% [b] (sediment)	84 days	EU 2001e
ZK 512723	pyrimethanil	6.1 - 10.4%	100 days	PSD 1995k
BH518-2	quinmerac	<1%	-	PSD 1998c
BH518-5	quinmerac	<1%	-	PSD 1998c
3-hydroxyquioxyfen	quinoxyfen	41% [g]	-	Roberts and Hutson 1999
6-hydroxyquioxyfen	quinoxyfen	10% [g]	100 days	Roberts and Hutson 1999
IN-70941	rimsulfuron	main [g]	-	PSD 1996f
IN-70942	rimsulfuron	main [g]	-	PSD 1996f
IN-E9260	rimsulfuron	<7%	-	PSD 1996f
IN-J290	rimsulfuron	<7%	21 days	PSD 1996f
deisopropylatrazine	simazine	6.3 - 7.2% (water)	77 days	PSD 1992e
		0.4 - 1.4% (sediment)	77 days	PSD 1992e
diaminochlorotriazine, deisopropyl hydroxystrzine and hydroxydideethylsimazine combined	simazine	3.3 - 3.9% (water)	77 days	PSD 1992e
sulfosulfuron desmethyl	sulfosulfuron	13%	-	PMRA 1998

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Sediment /water systems continued...				
sulfonamide	sulfosulfuron	major [g] (anaerobic)	-	PMRA 1998
aminopyrimidine	sulfosulfuron	major [g] (anaerobic)	-	PMRA 1998
anilino acid	tau-fluvalinate	20 - 27% [b] (whole system)	-	PSD 1997e
		13 - 19% (water)	-	PSD 1997e
haloaniline	tau-fluvalinate	9.5% [b]	-	PSD 1997e
dicarboxylic acid	tau-fluvalinate	<1.5%	-	PSD 1997e
3-phenoxybenzoic acid	tau-fluvalinate	15% [b] (whole system)	-	PSD 1997e
		10% (water)	-	PSD 1997e
RH-96595	tebufenozide	major [g]	-	PMRA 1996b
RH-112703	tebufenozide	major [g]	-	PMRA 1996b
RH-112651	tebufenozide	major [g]	-	PMRA 1996b
AC 810 723	tebufenpyrad	9 - 17%	60 - 100 days	PSD 1995o
DP-1	tepraloxydim	11%	-	PMRA 2004b
		12.1% (anaerobic)		PMRA 2004b
DP-6	tepraloxydim	minor [g]	-	PMRA 2004b
		minor [g] (anaerobic)	-	PMRA 2004b
DP-2	tepraloxydim	minor [g] (anaerobic)	-	PMRA 2004b
GS 26379	terbuthylazine	6.62%	22 days	PSD 1993a
GS 23158	terbuthylazine	8.72%	30 days	PSD 1993a
thifensulfuron acid	thifensulfuron-methyl	80% [b] (water)	91 days	EU 2001g
		32% [b] (sediment)	91 days	EU 2001g
		30% [b] (anaerobic, whole system)	56 days	EU 2001g
		55% [b] (water)	70 days	EU 2001g
		60 - 87% [b] (water)	13 weeks	PSD 1995n
		minor [g] (anaerobic)	-	PSD 1991i
2-acid-3-sulfonamide	thifensulfuron-methyl	42% [b] (water)	56 days	EU 2001g
		37% b (anaerobic, whole system)	196 days	EU 2001g
		39% [b] (water)	182 days	EU 2001g
		major [g] (anaerobic)	-	PSD 1991i
2-ester-3-sulfonamide	thifensulfuron-methyl	40% [b] (anaerobic, whole system)	112 days	EU 2001g
		major [g] (anaerobic)	-	PSD 1991i
2-acid-3-sulfonic acid	thifensulfuron-methyl	24% [b] (anaerobic, whole system)	196 days	EU 2001g
		major [g] (anaerobic)	-	PSD 1991i
O-demethyl thifensulfuron acid	thifensulfuron-methyl	21% [b] (water)	125 days	EU 2001g
		minor [g] (anaerobic)	-	PSD 1991i
triazine urea	thifensulfuron-methyl	25% [b] (water)	182 days	EU 2001g
IN-A4098	thifensulfuron-methyl	19% [b] (water)	-	EU 2001g
3-aminosulfonyl-2-thiophene carboxylic acid	thifensulfuron-methyl	40% [b] (water)	8 weeks	PSD 1995n
2-ester-triuret	thifensulfuron-methyl	minor [g] (anaerobic)	-	PSD 1991i
4-chlorobezoic acid	thiobencarb	14.2%	-	EPA 1997e
methomyl	thiodicarb	7.2% (anaerobic)	0 days	EPA 1998k
acetonitrile	thiodicarb	72.5%	14 days	EPA 1998k
carbendazim	thiophanate-methyl	66% (anaerobic)	1 days	EPA 2001c
AV-1951	thiophanate-methyl	<10% (anaerobic)	-	EPA 2001c
DX-105	thiophanate-methyl	<10% (anaerobic)	-	EPA 2001c
FH-432	thiophanate-methyl	<10% (anaerobic)	-	EPA 2001c
DMST	tolyfluanid	72.7% [b] (water)	14 days	PSD 1995q
		28.5% [b] (sediment)	30 days	PSD 1995q

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Sediment /water systems continued...				
RNH 0189	tolyfluanid	6.1% [b] (water)	75 days	PSD 1995q
		1.6% [b] (sediment)	120 days	PSD 1995q
tralkoxydim metabolite 9	tralkoxydim	10.7% [b] (water)	14 days	PSD 1993m
		<6% (anaerobic, water)	-	PSD 1993m
		22.2% [b] (sediment)	90 days	PSD 1993m
		35 - 39% (anaerobic, sediment)	119 days	PSD 1993m
tralkoxydim metabolite 8	tralkoxydim	11.2% [b] (water)	30 days	PSD 1993m
		<6% (anaerobic, water)	-	PSD 1993m
		2.7% (sediment)	14 days	PSD 1993m
		<5% (anaerobic, sediment)	-	PSD 1993m
tralkoxydim metabolite 10	tralkoxydim	2.9% [b] (water)	119 days	PSD 1993m
		<6% (anaerobic, water)	-	PSD 1993m
		1% (sediment)	0 days	PSD 1993m
		<5% (anaerobic, sediment)	-	PSD 1993m
CGA 150829	triasulfuron	10 - 11% (water)	10 weeks	EU 2000d
		0.3% (anaerobic, water)	70 days	EU 2000d
O-desmethyl triasulfuron	triasulfuron	5 - 13% (water)	10 weeks	EU 2000d
chlorosulfonamide	triasulfuron	<10% (water)	10 weeks	EU 2000d
triazamate metabolite X	triazamate	45 - 47% (water)	2 days	PSD 1998d
triazamate metabolite II	triazamate	18 - 25% (water)	30 days	PSD 1998d
triazmate metabolite XVII	triazamate	38 - 49% (water)	14 days	PSD 1998d
		5 -8% (sediment)	59 days	PSD 1998d
triazamte metabolite XI	triazamate	16 - 23% (water)	59 days	PSD 1998d
		9 - 12% (sediment)	14 days	PSD 1998d
triazmate metabolite III	triazamate	4% (water)	-	PSD 1998d
triazamte metabolite IX	triazamate	2% (water)	-	PSD 1998d
SAS 9256	triazoxide	42.1 - 48.5% (whole system)	30 days	PSD 1993n
SAS 10942	triazoxide	3.5 - 11.3% (whole system)	-	PSD 1993n
acid sulphonamide A	tribenuron methyl	12 - 28% (anaerobic)	24 days	PSD 1992h
		19% [g] (water)	56 days	EFSA 2004
saccharin	tribenuron methyl	70 - 73% (anaerobic)	24 days	PSD 1992h
		32% [g] (water)	14 days	EFSA 2004
O-demethyl tribenuron methyl acid	tribenuron methyl	19%	4 weeks	PSD 1992h
triazine amine A	tribenuron methyl	61 - 71% (anaerobic)	24 days	PSD 1992h
		34.8%	4 weeks	PSD 1992h
		42% [g] (water)	14 days	EFSA 2004
		86% [g] (sediment)	56 days	EFSA 2004
3,5,6-trichloro-2-pyridinol	triclopyr	25% (anaerobic, water)	365 days	EPA 1998l
		<5%	30 days	EPA 1998l
CGA-321113	trifloxystrobin	major [g]	-	PMRA 2004h
CGA-331409	trifloxystrobin	minor [g]	-	PMRA 2004h
methyl saccahrin	triflusulfuron-methyl	25 - 38% (water)	-	PSD 1995r
methyl saccahrin and unidentified metabolite combined	triflusulfuron-methyl	12% (sediment)	100 days	PSD 1995r
triflusulfuron-methyl acid	triflusulfuron-methyl	45%	100 days	PSD 1995r
triazine amine B	triflusulfuron-methyl	42.1%	30 days	PSD 1995r
N-demethyl triazine amine B	triflusulfuron-methyl	10 - 15%	-	PSD 1995r
trinexapac acid	trinexapac ethyl	48 - 64%	14 days	PSD 1995s
		major [g]	-	PMRA 2001b
pyrithione disulfide	zinc pyrithione	16.9% (whole system)	7 days	HSE 2003b
		28.07% (anaerobic, whole system)	3 days	HSE 2003b
pyrithione sulfinic acid	zinc pyrithione	16.5% (whole system	1 day	HSE 2003b

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Sediment /water systems continued...				
		13.47% (anaerobic, whole system)	0.25 days	HSE 2003b
pyridine sulfinic acid	zinc pyrithione	31.98% (anaerobic, whole system)	90 days	HSE 2003b
pyridine sulfonic acid	zinc pyrithione	22.75% (anaerobic, whole system)	0.75 days	HSE 2003b
RH-163353	zoxamide	major [g]	-	PMRA 2001d
RH-127450	zoxamide	major [g]	-	PMRA 2001d
Aqueous photolysis				
1,2,4-benzenetriol	2,4-D	>10%	-	PSD 1993a
		31.7%	30 days	EU 2001a
2,6-diethyl-N-methoxymethyl acetanilide	alachlor	≤1.57%	30 days	EPA 1998b
dihydroxy anilazine	anilazine	86.9%	364 hours	PSD 1994b
deethylatrazine	atrazine	2.8%	15 days	Solomon et al. 1996
		38%	7 days	PSD 1992b
		<4%	-	APVMA 1997a
hydroxyatrazine	atrazine	2.6%	15 days	Solomon et al. 1996
		14.6%	7 days	PSD 1992b
		<4%	-	APVMA 1997a
deisopropylatrazine	atrazine	1.2%	6.9 days	Solomon et al. 1996
		4.3%	7 days	PSD 1992b
		<4%	-	APVMA 1997a
diaminochloroatrazine	atrazine	22%	7 days	PSD 1992b
		0.9%	15 days	Solomon et al. 1996
		<4%	-	APVMA 1997a
DIHA	atrazine	1.2%	6.9 days	Solomon et al. 1996
		<4%	-	APVMA 1997a
DEHA	atrazine	0.4%	15 days	Solomon et al. 1996
		<4%	-	APVMA 1997a
reference compound 28	azoxystrobin	minor [g]	-	PMRA 2000a
reference compound 30	azoxystrobin	minor [g]	-	PMRA 2000a
3-isopropyl-2,3-dioxo-5-oxocyclo-penteno[d]1H-2,1,3-thiadiazin-4(3H)-one 6-carbonic acid	bentazone	21% (pH 7)	-	EU 2000a
		21% (pH 7)	142 hours	EPA 2001a
1-[N-(1-methyl-ethyl)]-1-sulfoamino-benzamide	bentazone	6.46% (pH 7)	142 hours	EPA 2001a
1,2,4-triazole	bitertanol	52.5%	-	PSD 1994c
4-hydroxybiphenyl	bitertanol	12.0%	-	PSD 1994c
3-bromo-4-hydroxy-benzonitrile	bromoxynil	major [g]	-	EU 2004d
4-hydroxy-benzonitrile	bromoxynil	major [g]	-	EU 2004d
bromoxynil	bromoxynil octanoate	major [g]	-	EU 2004d
4-cyano-2-bromophenyl octanoate	bromoxynil octanoate	13.9% [b]	3 days	EPA 1998c
3,5,-dibromo-4-hydroxybenzonitrile	bromoxynil octanoate	53.4% [b]	30 days	EPA 1998c
phenyl carbamate	bromoxynil octanoate	26.6% [b]	2 days	EPA 1998c
DNTBA	butralin	31.8%	11 days	PSD 1998a
4-hydroxy-2,5,6-trichloroisophthalonitrile	chlorothalonil	10%	-	EPA 1999b
2-amino-4-methoxy-6-methyl-1,3,5-triazine	chlorsulfuron	5 - 44%	-	PSD 1991a
2-chlorobenzene sulfonamide	chlorsulfuron	4 - 21%	-	PSD 1991a
2-chlorophenylsulfonyl urea	chlorsulfuron	0 - 4%	-	PSD 1991a
O,O-diethyl-O-(3-acetoxy) phenylphosphorothioate	coumaphos	43%	83.5 hours	EPA 1996d
coumaphoxon	coumaphos	10.2%	-	EPA 1996d
CCIM	cyazofamid	39.6% [g]	6 hours - 2 days	EU 2002e
HTID	cyazofamid	18.5% [g]	21 days	EU 2002e
p-toluamide	cyazofamid	12.1% [g]	36 days	EU 2002e
CCTS	cyazofamid	37.9% [g]	3 - 6 hours	EU 2002e
T1S	cycloxydim	10 - 45% (pH 5.5)	-	PSD 1990b
		6 - 43% (pH 9.4)	-	PSD 1990b
T2S	cycloxydim	3 - 9% (pH 5.5)	-	PSD 1990b
		2 - 7% (pH 9.4)	-	PSD 1990b
TSO	cycloxydim	6 - 11% (pH 5.5)	-	PSD 1990b
TSO_2 and $T2SO_2$ combined	cycloxydim	< 3% (pH 5.5)	-	PSD 1990b
TSO and T2SO combined	cycloxydim	2 - 8% (pH 9.4)	-	PSD 1990b
4-fluoro-3-phenoxybenzoic acid	cyfluthrin	37%	14 days	EU 2002c
4-fluoro-3-phenoxybenzaldehyde	cyfluthrin	12%	14 days	EU 2002c
DCVA	cyfluthrin	>10%	-	EU 2002c
compound Ia	*lambda*-cyhalothrin	major [g]	-	EU 2001d

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Aqueous photolysis continued...				
3-phenoxybenzoic acid	*lambda*-cyhalothrin	14%	-	PMRA 2003d
		major [g]	-	EU 2001d
		25%	-	PMRA 2003d
aminooxacetic acid	cymoxanil	minor [g]	-	PMRA 2000b
JX915	cymoxanil	52%	-	PMRA 2000b
U3204	cymoxanil	minor [g]	-	PMRA 2000b
T4226	cymoxanil	minor [g]	-	PMRA 2000b
KP533	cymoxanil	minor [g]	-	PMRA 2000b
R3273	cymoxanil	35%	-	PMRA 2000b
CGA 272749	cyprodinil	19% (pH 7.3)	-	PSD 1997a
CGA 2249287	cyprodinil	~16% (pH 7.3)	-	PSD 1997a
phenylguanidine	cyprodinil	1% (pH 7.3)	-	PSD 1997a
3-phenoxybenzoic acid	deltamethrin	main [g]	-	EU 2002g
ethyl-m-hydroxyphenyl carbamate	desmedipham	5% (pH 3.8)	-	PSD 1993d
		10% (pH 3.8)	10 hours	EPA 1996e
ethyl N-(3-hydroxy-4-phenyl	desmedipham	<1%	-	EPA 1996e
ethyl N-(2-phenylcarbamyl-5-hydroxyphenyl) carbamate	desmedipham	<1%	-	EPA 1996e
4-chloro-2(3H)benzoxazolone	diclobenil	17%	21 days	EPA 1998e
2-hydroxybenzonitrile	diclobenil	4%	21 days	EPA 1998e
2,6-dichlorobenzoic acid	diclobenil	3%	21 days	EPA 1998e
2-chlorobenzonitrile	diclobenil	2%	21 days	EPA 1998e
2,6-dichlorobenzamide	diclobenil	1%	21 days	EPA 1998e
4-hydroxy-2,6-dichlorobenzonitrile	diclobenil	1%	21 days	EPA 1998e
o,p'-dichlorobenzophenone	o,p'-dicofol	major [g]	-	EPA 1998f
p,p'-dichlorobenzophenone	p,p'-dicofol	major [g]	-	EPA 1998f
4-(2,4-dichlorophenoxy)phenol	diclofop-methyl	0 - 33%	237 - 288 hours	PSD 1995b
EPTC sulfoxide	EPTC	3.4%	-	EPA 1999c
EPTC sulfone	EPTC	2%	-	EPA 1999c
N,N-dipropylformamide	EPTC	1.9%	-	EPA 1999c
dipropylamine	EPTC	35.7%		EPA 1999c
s-trifluoromethyl-3-nitro-1,2-benzendiamine	ethalfluralin	24.4%	-	PSD 1995l
Cl-Vacid	esfenvalerate	17.3%	10 days	PSD 1992c
IN-JS940	famoxadone	major [g]	-	PMRA 2003h
IN-H3310	famoxadone	major [g]	-	PMRA 2003h
IN-JL856	famoxadone	minor [g]	-	PMRA 2003h
IN-KF015	famoxadone	minor [g]	-	PMRA 2003h
WAK 7004	fenhexamid	24%	1 hour	PMRA 2003b
hydroxylated fenhexamid	fenhexamid	major [g]	15 days	PMRA 2003b
succinic acid	fenhexamid	major [g]	15 days	PMRA 2003b
p-nitro-m-cresol	fenitrothion	major [g]	-	PMRA 1993a
carboxy-fenitrothion	fenitrothion	10% (pH 5)	14 days	APVMA 1999
0,0-dimethyl 0-(3-carboxyl-4-nitro-phenyl) phosphorothioate	fenitrothion	12.4% [b]	14 - 30 days	EPA 1995c
fenoxaprop-ethyl acid	fenoxaprop-ethyl	6.9%	192 hours	PSD 1990c
4-(6-chloro-2-benzoxazolyloxy)phenol	fenoxaprop-ethyl	6.4%	192 hours	PSD 1990c
Ro 43-4755	fenoxycarb	12.3%	360 minutes	PSD 1997b
3-phenoxybenzoic acid	fenpropathrin	11 – 39%	6 weeks	PSD 1989a
2,2,3,3-tetramethyl cyclopropane carboxylic acid	fenpropathrin	2 – 39%	6 weeks	PSD 1989a
α-(2,2,3,3-tetramethylcyclopropyl)-3-phenoxybenzyl cyanide	fenpropathrin	5 – 13%	6 weeks	PSD 1989a
α-carbomoyl-3-phenoxybenzyl-2,2,3,3-tetramethyl cyclopropane carboxylate	fenpropathrin	4 - 28%	6 weeks	PSD 1989a
M3 and M4 combined	fenpyroximate	10%	24 hours	PSD 1995d
1,3-dimethyl-5-phenoxypyrazole-4-carbonitrile	fenpyroximate	47.5 - 58.3%	6 hours	PSD 1995d
MB 46513	fipronil	43%	6 hours	PSD 2004a
RPA 104615	fipronil	8.2%	6 hours	PSD 2004a
triazolopyrimidine sulphonic acid-florasulam	florasulam	17%	-	PMRA 2004a
compound V	fluazinam	51% (pH 9)	30 days	PSD 1994i
		minor (pH 5)	30 days	PSD 1994i
MKH 6562 sulfonamide	flubcarbazone-sodium	22.6%	-	PMRA 2000c
MKH 6562 sulfonic acid	flubcarbazone-sodium	1.32%	-	PMRA 2000c
2,6-difluorobenzamide	flufenoxuron	>40%	31 days	HSE 1995
1-(2,6-difluorobenzoyl)-3-(4-hydroxyphenyl) urea	flufenoxuron	5.5%	31 days	HSE 1995
RH-4514	fluoroglycofen-ethyl	5.8%	-	PSD 1992d
1H-1,2,4-triazole	flusilazole	<5%	30 days	PSD 1989b

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Aqueous photolysis continued...				
4-(3-carboxyphenyl)-5-methyl amino-2-phenyl -furan-3(2H)-one	flurtamone	33.5%	-	PSD 2000a
3-methyl phosphinico-proprionic acid	glufosinate ammonium	19% (pH 9)	120 hours	PSD 1990f
1,5-bis(α,α,α-p-tolyl)-1,4-pentadien-3-one	hydramethylnon	<8%	90 minutes	PSD 1994j
TDTP	hydramethylnon	<8%	90 minutes	PSD 1994j
α,α,α-trifluoro-p-toluic acid	hydramethylnon	<8%	90 minutes	PSD 1994j
p-trifluoromethyl cinnamic acid	hydramethylnon	<8%	90 minutes	PSD 1994j
quinoline-3-carboxylic acid	imazaquin	14%	24 hours	PSD 1993h
2H-azolidino[3,4-b]quinoline-1,3-dione	imazaquin	21%	48 hours	PSD 1993h
3-imino-2H-azolidino[3,4-b]quinolin-1-one	imazaquin	13%	48 hours	PSD 1993h
quinoline-2,3-dicarboxylic acid	imazaquin	~30%	48 hours	PSD 1993h
AE 0002166	iodosulfuron-methyl	major [g]	-	PMRA 2004f
ioxynil	ioxynil octanoate	major [g]	-	EU 2004g
4-hydroxybenzonitrile	ioxynil octanoate	major [g]	-	EU 2004g
4-cyano-2-idophenyl octanaote	ioxynil octanoate	major [g]	-	EU 2004g
3-iodo-4-hydroxybenzonitrile	ioxynil octanoate	minor	-	EU 2004g
3,5-di-iodo-4-hydroxybenzamide	ioxynil octanoate	minor	-	EU 2004g
3-(4-isopropyl phenyl)-1-methylurea	isoproturon	5%	24 hours	PSD 1995g
4-isopropyl phenylurea	isoproturon	3%	24 hours	PSD 1995g
4-isopropyl aniline	isoproturon	4%	24 hours	PSD 1995g
4-aminophenol	isoproturon	26%	78 hours	PSD 1995g
malonic acid	kathon 886	>20%	-	HSE 1993
N-methyl malonamic acid	kathon 886	>20%	-	HSE 1993
malonamic acid	kathon 886	>20%	-	HSE 1993
acetic acid	kathon 886	<20%	-	HSE 1993
formic acid	kathon 886	<20%	-	HSE 1993
S-(1,2-di(carbethoxy)ethyl)-0-methyl hydrogen phosphorodithioate	malathion	10 - 20% (pH 4)	30 days	PSD 1995l
2-methyl-4-chlorophenol	MCPA	11.6%	-	EU 2005j
o-cresol	MCPB	18% (pH 5)	-	EU 2005k
		48.5% (pH 7)	-	EU 2005k
		26.2% (pH 9)	-	EU 2005k
4-(4-hydroxy-o-tolyloxy)butyric acid	MCPB	33% (pH 5)	-	EU 2005k
		28.5% (pH 7)	-	EU 2005k
		17.8% (pH 9)	-	EU 2005k
2,4 dihydroxyphenyl formate	MCPB	41.6% (pH 5)	-	EU 2005k
		36.5% (pH 7)	-	EU 2005k
		23.2% (pH 9)	-	EU 2005k
benzoic acid	MCPB	13.8% (pH 5)	-	EU 2005k
		1.6% (pH 7)	-	EU 2005k
		7.4% (pH 9)	-	EU 2005k
2-hydroxyphenyl formate	MCPB	10.4% (pH 5)	-	EU 2005k
		4.9% (pH 7)	-	EU 2005k
		14.4 (pH 9)	-	EU 2005k
CGA-62826	metalaxyl	6.1%	28 days	EPA 1994c
hydroxymetconazole	metconazole	14.5%	30 days	PSD 2000b
dechlorometconazole	metconazole	7.8%	30 days	PSD 2000b
methiocarb sulfoxide	methiocarb	9.8%	30 days	PSD 1998b
methiocarb sulfoxide phenol	methiocarb	2.7%	30 days	PSD 1998b
acetonitrile	methomyl	66%	15 days	EPA 1998h
S-methyl-N-hydroxythioacetimidate	methomyl	≤3%	-	EPA 1998h
methyl-2-(aminosulfonyl)benzoate	metsulfuron-methyl	58% (dark)	14 days	PSD 1991e
		13%	4 days	PSD 1991e
saccharin	metsulfuron-methyl	7%	14 days	PSD 1991e
2-(aminosulfonyl) benzoic acid	metsulfuron-methyl	7%	14 days	PSD 1991e
ASDM	nicosulfuron	60.9% (pH 4.9)	-	PSD 2000c
		3.5% (pH 7.3)	-	PSD 2000c
		2.7% (pH 9.2)	-	PSD 2000c
		23.1% (pH 5)	-	PSD 2000c
		3.1% (pH 9)	-	PSD 2000c
DPSA	nicosulfuron	1.6% (pH 9.2)	-	PSD 2000c
DMPU	nicosulfuron	2.1% (pH 5)	-	PSD 2000c
		1.6% (pH 9)	-	PSD 2000c
3-nitro-5-aminosulfanilamide	oryzalin	2.9%	12 hours	EPA 1994d
3-nitro-5-amino-N-propylsulfanilamide	oryzalin	4%	12 hours	EPA 1994d
3,5-dinitro sulfanilamide	oryzalin	5.7%	12 hours	EPA 1994d
2-ethyl-7-nitro-1-propyl-5-sulfonylaminobenzimidazole 3-oxide	oryzalin	14%	12 hours	EPA 1994d
2-chloro-1-(3-ethoxy-4-hydroxyphenol)-4-(trifluoromethyl) benzene	oxyfluorfen	>10%	-	PSD 1996a
4-carboxy-1-methylpyridinium	paraquat	6%	85 weeks	EPA 1997c

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Aqueous photolysis continued...				
2,6-dinitro-3,4-dimethyl aniline	pendimethalin	9.3%	-	EPA 1997d
phorate sulfoxide	phorate	major [g]	-	PMRA 2003a
phorate sulfone	phorate	major [g]	-	PMRA 2003a
formaldehyde	phorate	major [g]	-	PMRA 2003a
5,6-dimethyl-2-dimethylamino-pyrimidin-4-ol	pirimicarb	20% (pH 5)	8 days	PSD 1994m
		16% (pH 7)	8 days	PSD 1994m
		24% (pH 9)	8 days	PSD 1994m
5,6-dimethyl-2-methylamino-4-pyrimidin-4-ol, 2-amino-5,6-dimethyl-pyrimidin-4-ol and guanidine combined	pirimicarb	<5% (pH 5)	8 days	PSD 1994m
		<5% (pH 7)	8 days	PSD 1994m
		<1% (pH 9)	8 days	PSD 1994m
5,6-dimethyl-2-methylamino-pyrimidin-4-yl-dimethylcarbamate	pirimicarb	4% (pH 5)	8 days	PSD 1994m
		6% (pH 7)	8 days	PSD 1994m
		3% (pH 9)	8 days	PSD 1994m
5,6-dimethyl-2-methylformamido-pyrimidin-4-yl-dimethyl carbamate	pirimicarb	16% (pH 5)	8 days	PSD 1994m
		18% (pH 7)	8 days	PSD 1994m
		10% (pH 9)	8 days	PSD 1994m
didesmethyl pirimicarb	pirimicarb	11% (pH 5)	8 days	PSD 1994m
		9% (pH 7)	8 days	PSD 1994m
		17% (pH 9)	8 days	PSD 1994m
N,N-dimethylguanidine	pirimicarb	17% (pH 5)	8 days	PSD 1994m
		22% (pH 9)	8 days	PSD 1994m
N-methylguanidine	pirimicarb	20% (pH 5)	8 days	PSD 1994m
		10% (pH 9)	8 days	PSD 1994m
N,N-dimethylguanidine and N-methylguanidine combined	pirimicarb	36% (pH 7)	8 days	PSD 1994m
CGA-120844	primisulfuron methyl	54.6%	-	PMRA 2001a
saccharin	primisulfuron methyl	10.2%	-	PMRA 2001a
CGA-191429	primisulfuron methyl	0.7%	-	PMRA 2001a
CGA-171683	primisulfuron methyl	2%	-	PMRA 2001a
Ro 16-1976	propaquizafop	4.1%	3 days	PSD 1994n
Ro 41-0812	propaquizafop	1.2%	3 days	PSD 1994n
Ro 19-6241	propaquizafop	3.3%	3 days	PSD 1994n
hydroxylamine derivative	propaquizafop	6%	3 days	PSD 1994n
isopropoxy phenol	propoxur	major [g]	-	PSD 1993b
beta-(3,5-dichlorobenzamido)-*beta*-mebutyric acid	propyzamide	15%	-	EU 2003q
CGA 215525	pymetrozine	78.8%	-	PMRA 2002
CGA 249257	pymetrozine	38.8%	-	PMRA 2002
hydroxyl CGA 215525	pymetrozine	10.2%	-	PMRA 2002
CGA 294849	pymetrozine	5.3%	-	PMRA 2002
500M78	pyraclostrobin	major [g]	-	PMRA 2003n
BF 500-14	pyraclostrobin	major [g]	-	PMRA 2003n
500M58	pyraclostrobin	major [g]	-	PMRA 2003n
BF 500-13	pyraclostrobin	major [g]	-	PMRA 2003n
BF 500-11	pyraclostrobin	major [g]	-	PMRA 2003n
		37%	-	PMRA 2003n
2-(2-pyridyloxy) propyl alcohol	pyriproxyfen	15.8 - 30.4%	35 days	PSD 1996d
2-chloro-10-fluoro[1]benzopyrano[2,3,4-de]quinoline	quinoxyfen	30% [g]	-	Roberts and Hutson 1999
5,7-dichloro-4-hydroxyquinoline	quinoxyfen	11% [g]	-	Roberts and Hutson 1999
IN-70941	rimsulfuron	23.2 - 25.1%	21 days	PSD 1996f
IN-70942	rimsulfuron	6.9 - 9.8%	21 days	PSD 1996f
IN-E9260	rimsulfuron	16.2%	21 days	PSD 1996f
IN-J290	rimsulfuron	19.1%	21 days	PSD 1996f
aminopyrimidine	sulfosulfuron	major [g]	-	PMRA 1998
sulfamic acid	sulfosulfuron	major [g]	-	PMRA 1998
N-hydroxyl urea	sulfosulfuron	major [g]	-	PMRA 1998
oxamic acid	sulfosulfuron	major [g]	-	PMRA 1998
sulfonic acid	sulfosulfuron	major [g]	-	PMRA 1998
sulfone	sulfosulfuron	major [g]	-	PMRA 1998
anilino acid	tau-fluvalinate	9%	10 minutes	PSD 1997e
haloaniline	tau-fluvalinate	<5%	-	PSD 1997e
dicarboxylic acid	tau-fluvalinate	<5%	-	PSD 1997e
3-phenoxybenzoic acid	tau-fluvalinate	9.7% [b]	7 minutes	PSD 1997e
3-phenoxybenzaldehyde	tau-fluvalinate	<5%	-	PSD 1997e
cyanohydrin	tau-fluvalinate	10.7%	10 minutes	PSD 1997e
JA-231-2	tebuconazole	8 - 38%	-	PSD 1993k
		40%	-	PSD 1993k
		<3%	-	PSD 1993k

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Aqueous photolysis continued...				
KFE 1224	tebuconazole	11 - 21%	-	PSD 1993k
		7%	-	PSD 1993k
		5 - 6%	-	PSD 1993k
HWG 3877	tebuconazole	<2%	-	PSD 1993k
		<3%	-	PSD 1993k
HWG 2061	tebuconazole	<2%	-	PSD 1993k
		<3%	-	PSD 1993k
JA-230-4	tebuconazole	<2%	-	PSD 1993k
		<3%	-	PSD 1993k
JA-230-5	tebuconazole	<2%	-	PSD 1993k
		<3%	-	PSD 1993k
1,2,4-triazole	tebuconazole	0.6 - 14%	-	PSD 1993k
		<3%	-	PSD 1993k
DP-1	tepraloxydim	50% (pH 5)	-	PMRA 2004b
DP-2	tepraloxydim	19% (pH 7)	-	PMRA 2004b
GP	tepraloxydim	20% (pH 5)	-	PMRA 2004b
DP-6	tepraloxydim	13% (pH 9)	-	PMRA 2004b
2-tert-butylamino-4-chloro-6-amino-5-triazine	terbuthylazine	3.61%	-	PSD 1993a
tetraconazole dihydro isoquinoline triazole	tetraconazole	9.3% [b]	4 days	PSD 1999c
tetraconazole alcohol	tetraconazole	7.3% [b]	30 days	PSD 1999c
tetrafluoroethoxy triazolyl isobutanoic acid	tetraconazole	10.3% [b]	30 days	PSD 1999c
1,2,4-triazole	tetraconazole	7% [b]	22 days	PSD 1999c
benzimidazole-2-carboxamide	thiabendazole	10.22%	-	EU 2001f
IN-A4089	thifensulfuron-methyl	11%	-	PSD 1988c
		11.3%	48 days	PSD 1991i
thifensulfuron-methyl triazine urea	thifensulfuron-methyl	14%	-	PSD 1988c
		14.1%	48 days	PSD 1991i
thifensulfuron-methyl TP1	thifensulfuron-methyl	7%	-	PSD 1988c
		7.1 - 7.4%	48 days	PSD 1991i
4-chlorobezoic acid	thiobencarb	56%	-	EPA 1997e
4-chlorobenzaldehyde	thiobencarb	29.4%	-	EPA 1997e
4-chlorobenzyl alcohol	thiobencarb	6.1 - 6.7%	14 - 30 days	EPA 1997e
thiobencarb sulfoxide	thiobencarb	5%	14 days	EPA 1997e
O-[(4-chlorophenyl)methyl]diethyl carbamate	thiobencarb	17.7%	21 days	EPA 1997e
methomyl methylol	thiodicarb	1.95%	24 days	PSD 1992f
methomyl	thiodicarb	46.7%	24 days	PSD 1992f
		47% (pH 6)	23 days	EPA 1998k
methomyl oxime	thiodicarb	1.7%	24 days	PSD 1992f
UC54170	thiodicarb	5%	24 days	PSD 1992f
UC54171	thiodicarb	3%	24 days	PSD 1992f
carbendazim	thiophanate-methyl	49.7%	5.5 days	EPA 2001c
DX-105	thiophanate-methyl	14.3%	5.5 days	EPA 2001c
		4%	5.5 days	EU 2005m
FH-432	thiophanate-methyl	4.4%	5.5 days	EPA 2001c
ph-CH3	tolclofos-methyl	0.51% (pH 5)	30 days	PSD 1993l
		0.66% (pH 7)	14 days	PSD 1993l
		0.78% (pH 9)	14 days	PSD 1993l
TMO	tolclofos-methyl	8.16% (pH 5)	30 days	PSD 1993l
		11.97% (pH 7)	30 days	PSD 1993l
		12.02% (pH 9)	14 days	PSD 1993l
DM-TM	tolclofos-methyl	23.1% (pH 5)	30 days	PSD 1993l
		16.08% (pH 7)	30 days	PSD 1993l
		11.24% (pH 9)	30 days	PSD 1993l
tralkoxydim metabolite II	tralkoxydim	22%	59.7 days	PSD 1993m
tralkoxydim metabolite 10	tralkoxydim	22%	14.9 days	PSD 1993m
tralkoxydim metabolite IV	tralkoxydim	6.3%	89.5 days	PSD 1993m
CGA 183859 sulfonic acid derivative	triasulfuron	12.9% [b] (pH 9)	-	EU 2000d
triazine amine A	tribenuron methyl	6.5% (pH 9)	716 hours	PSD 1992h
N-demethyl triazine amine A	tribenuron methyl	3.8% (pH 9)	716 hours	PSD 1992h
O-demethyl triazine amine A	tribenuron methyl	1.1% (pH 9)	716 hours	PSD 1992h
sulphonamide A	tribenuron methyl	2.2% (pH 9)	716 hours	PSD 1992h
saccharin and acid sulphonamide A	tribenuron methyl	3.5% (pH 9)	716 hours	PSD 1992h
3,5,6-trichloro-2-pyridinol	triclopyr	principal [g]	-	PMRA 1991b
5-chloro-3,6-dihydroxy-2-pyridinoloxyacetic acid	triclopyr	48% (sterile)	-	EPA 1998l
oxamic acid	triclopyr	16%	-	EPA 1998l
5/6-chloro-3-hydroxy-s-pyridinone	triclopyr butoxyethyl ester	17%	30 days	EPA 1998l
dichloropyridinyloxyacetic acid	triclopyr butoxyethyl ester	6%	30 days	EPA 1998l

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Aqueous photolysis continued...				
2-hydroxy ethyl ester	triclopyr butoxyethyl ester	6%	30 days	EPA 1998l
CGA-357261	trifloxystrobin	major [g]	-	PMRA 2004h
2-ethyl-7-nitro-5-trifluoromethylbenzimidazole	trifluralin	47.4%	-	EPA 1996h
5-trifluoromethyl-3-nitro-1,2-benzene diamine	trifluralin	9.6%	-	EPA 1996h
2-ethyl-7-nitro-1-propyl-5-trifluoromethylbenzimidazole	trifluralin	53.8%	-	EPA 1996h
methyl saccahrin	triflusulfuron-methyl	71% [b] (pH 5)	-	PSD 1995r
		18 - 71%	-	PMRA 1999c
triazine amine B	triflusulfuron-methyl	47% [b] (pH 5)	-	PSD 1995r
		12 - 34%	-	PMRA 1999c
N-formyl methyl triazine amine B	triflusulfuron-methyl	20% [b] (pH 5)	-	PSD 1995r
		20%	-	PMRA 1999c
N-demethyl triazine amine B	triflusulfuron-methyl	7% [b] (pH 5)	-	PSD 1995r
N-demethyl triflusulfuron-methyl	triflusulfuron-methyl	15% [b] (pH 7)	-	PSD 1995r
		15%	-	PMRA 1999c
propane-1,2,3-tricarboxylic acid	trinexapac ethyl	major [g] (pH 5.1 & 7.4)	-	PSD 1995s
		56% (pH 7)	-	PSD 1995s
crotonyl CGA 163935	trinexapac ethyl	major [g] (pH 5.1 & 7.4)	-	PSD 1995s
		6% (pH 7)	-	PSD 1995s
RPA 406203	triticonazole	42%	6 days	PSD 2000d
		42 - 48%	-	PMRA 2004c
pyrithione sulfonic acid	zinc pyrithione	70.12% (pH 9)	30 days	HSE 2003b
pyrithione sulfinic acid	zinc pyrithione	<10% (pH 9)	30 days	HSE 2003b
		11.59% (pH 9)	30 days	HSE 2003b
dimethyl formamide	ziram	23.7%	24 hours	PSD 1994c
dimethylthioformamide	ziram	18.1%	24 hours	PSD 1994c
RH-150721	zoxamide	15%	-	PMRA 2001d
RH-24549	zoxamide	27.7%	-	PMRA 2001d
RH-139432	zoxamide	42.4%	-	PMRA 2001d
Hydrolysis (sterile)				
chloroallyl alcohol	1,2-dichloropropene	72% [b]	-	EPA 1998a
chloroallyl alcohol	1,3-dichloropropene	main [g]		EPA 1998a
alachlor oxamic acid	alachlor	2.2 - 25.1%	28 days	PSD 1990a
alachlor ethane sulfonic acid	alachlor	0.3 - 5.5%	28 days	PSD 1990a
2-amino-4,6-dimethoxypyrimidine	amidosulfuron	21% (pH 5)	30 days	PSD 1994a
		2% (pH 6)	30 days	PSD 1994a
product A (unidentified)	amidosulfuron	23%	30 days	PSD 1994a
BTS 27271	amitraz	primary [g]	-	EPA 1996a
BTS 27919	amitraz	primary [g]	-	EPA 1996a
BTS 24868	amitraz	secondary [g]	-	EPA 1996a
monohydroxy anilazine	anilazine	65.3% (pH 8.9)	52 hours	PSD 1994b
		52.1% (pH 7)	23 days	PSD 1994b
monohydroxy anilazine continued	anilazine	24.1% (pH 5)	12 days	PSD 1994b
dihydroxy anilazine	anilazine	0.19% (pH 8.9)	48 hours	PSD 1994b
		0.97% (pH 7)	23 days	PSD 1994b
		52.1% (pH 8.9)	18 days	PSD 1994b
reference compound 2	azoxystrobin	major [g]	-	PMRA 2000a
benalaxyl acid	benalaxyl	'main' [g]	-	EU 2004c
carbofuran	benfuracarb	54% (pH 7)	-	PSD 1998a
		9% (pH 9)	-	PSD 1998a
		13.6% (pH 7.1)	21.5 hours	PSD 1998a
carbofuran phenol	benfuracarb	35% (pH 7)	-	PSD 1998a
		76% (pH 9)	-	PSD 1998a
		10.7% (pH 7.1)	21.5 hours	PSD 1998a
N-hydroxy-methyl carbofuran	benfuracarb	24% (pH 7.1)	21.5 hours	PSD 1998a
bromoxynil	bromoxynil octanoate	35% (pH 5)	30 days	EU 2004d
		77.2% (pH 7)	30 days	EU 2004d
		76% (pH 9)	120 hours	EU 2004d
3,5-dibromo-dihdroxycyclohexadienylnitrile	bromoxynil octanoate	10.4% (pH 5)	21 days	EU 2004d
		10.7% (pH 7)	21 days	EU 2004d
3,5-dibromo-4-hydroxybenzonitrile	bromoxynil octanoate	35% [b] (pH 5)	30 days	EPA 1998c
		77% [b] (pH 7)	30 days	EPA 1998c
		76% [b] (pH 9)	30 days	EPA 1998c
3,5-dibromo-dihydroxy-cyclohexadienylnitrile	bromoxynil octanoate	10.4% [b] (pH 5)	-	EPA 1998c
		10.7% [b] (pH 7)	-	EPA 1998c
		7.9% [b] (pH 9)	-	EPA 1998c
1-tert-butyl-3-isopropyl-5-phenyl-2-biuret	buprofezin	42% (pH 4)	11 days	PSD 1993b
1-isopropyl-3-phenyl urea	buprofezin	15% (pH 4)	11 days	PSD 1993b

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Aqueous photolysis continued...				
4-hydroxy-2,5,6-trichloroisophthalonitrile	chlorothalonil	22% (pH 9)	49 days	PSD 2002
		11.3% (pH 9)	72 days	PSD 2002
		20% (pH 9)	89 days	EPA 1999b
3-cyano-2,4,5,6-tetrachlorobenzamide	chlorothalonil	54% (pH 9)	49 days	PSD 2002
		48.9% (pH 9)	72 days	PSD 2002
		50% (pH 9)	89 days	EPA 1999b
3,5,6-trichloro-2-pyridinol	chlorpyrifos	48% [b]	-	EPA 1999d
O-ethyl O-(3,5,6-trichloro-2-pyridinol) phosphorothioate	chlorpyrifos	13% [b]	-	EPA 1999d
deethyl chlorpyrifos	chlorpyrifos	main [g]	-	APVMA 2000b
cloquintocet acid	cloquintocet-mexyl	40 - 91%	-	PSD 1995a
chlorferon	coumaphos	4.3%	-	EPA 1996d
coumaphoxon	coumaphos	4.3%	-	EPA 1996d
6-hydroxy-3-methylbenzofuran	coumaphos	2.6% (pH 7)	-	EPA 1996d
CCIM	cyazofamid	79 - 82% (pH 5)	30 days	EU 2002e
CCIM	cyazofamid	83% (pH 7)	30 days	EU 2002e
CCIM	cyazofamid	74 -77% (pH 9)	30 days	EU 2002e
CCIM-AM	cyazofamid	10% (pH 9)	30 days	EU 2002e
TSO	cycloxydim	12 - 16% (pH 7)	32 days	PSD 1990b
		19% (pH 3)	0 days	PSD 1990b
		7 - 11% (pH 5)	14 days	PSD 1990b
		10 - 18% (pH 9)	7 days	PSD 1990b
T1S	cycloxydim	3 - 6% (pH 7)	32 days	PSD 1990b
		7% (pH 3)	30 minutes	PSD 1990b
		4 - 7% (pH 5)	14 days	PSD 1990b
		4% (pH 9)	7 days	PSD 1990b
T2S	cycloxydim	3 - 9% (pH 7)	32 days	PSD 1990b
		3% (pH 9)	7 days	PSD 1990b
T2SO	cycloxydim	10% (pH 3)	6 days	PSD 1990b
T2	cycloxydim	70% (pH 3)	6 days	PSD 1990b
		52% (pH 5)	14 days	PSD 1990b
4-fluoro-3-phenoxybenzaldehyde	cyfluthrin	89% (pH 9)	21 days	EU 2002c
		11% (pH 7)	35 days	EU 2002c
compound Ia	*lambda*-cyhalothrin	major [g]	-	EU 2001d
3-phenoxybenzaldehyde	*lambda*-cyhalothrin	major [g]	-	EU 2001d
aminooxacetic acid	cymoxanil	minor [g]	-	PMRA 2000b
JX915	cymoxanil	minor [g]	-	PMRA 2000b
W3595	cymoxanil	39% (pH 9)	-	PMRA 2000b
U3204	cymoxanil	60% (pH 9)	-	PMRA 2000b
KP533	cymoxanil	57% (pH 7)	-	PMRA 2000b
KQ960	cymoxanil	minor [g]	-	PMRA 2000b
R3273	cymoxanil	10% (pH 7)	-	PMRA 2000b
oxalic acid	cymoxanil	minor [g]	-	PMRA 2000b
3-phenoxybenzaldehyde	deltamethrin	main [g]	-	EU 2002g
decamthrinic acid	deltamethrin	trace	-	EU 2002g
diphenylurea	desmedipham	<0.6%	-	PSD 1993d
o,p'-dichlorobenzophenone	o,p'-dicofol	major [g]	-	EPA 1998f
2-chlorobenzoic acid	o,p'-dicofol	minor [g]	-	EPA 1998f
p,p'-dichlorobenzophenone	p,p'-dicofol	major [g]	-	EPA 1998f
M1	diflufenzopyr	major (pH 5)	-	PMRA 1999b
M6	diflufenzopyr	major (pH 5)	-	PMRA 1999b
N-demethyldimefuron	dimefuron	<10%	-	PSD 1993e
compound D	dimefuron	<10%	-	PSD 1993e
compound G	dimefuron	<10%	-	PSD 1993e
[(3-chlorophenyl)amino]-N,N-dimethylcarboxamide	dimefuron	<10%	-	PSD 1993e
[(3-chloro-4-hydroxyphenyl)amino]-N,N-dimethylcarboxamide	dimefuron	<10%	-	PSD 1993e
O-desmethyldimethoate	dimethoate	12% (pH 5)	30 days	PSD 1993f
		22% (pH 7)	30 days	PSD 1993f
		62% (pH 9)	30 days	PSD 1993f
O,O-dimethylphosphorothioic acid	dimethoate	ND (pH 5)	30 days	PSD 1993f
		2% (pH 7)	30 days	PSD 1993f
		36% (pH 9)	30 days	PSD 1993f
3,4-dichloroaniline	diuron	0.5% (pH 5, 7 & 9)	-	EPA 2003b
endosulfan diol	endosulfan	major [g]	-	EPA 2002c
Cl-Vacid	esfenvalerate	14.9% (pH 9)	28 days	PSD 1992c
CIPA	esfenvalerate	27%	7 days	EU 2000b
IN-JS940	famoxadone	major [g] (pH 5, 7 and 9)	-	PMRA 2003h
IN-JL856	famoxadone	major [g] (pH 7 and 9)	-	PMRA 2003h
IN-H3310	famoxadone	minor [g] (pH 5) major [g] (pH 7)	-	PMRA 2003h

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Aqueous photolysis continued...				
		minor [g] (pH 5 and 9)	-	PMRA 2003h
IN-MN968	famoxadone	major [g] (pH 9)	-	PMRA 2003h
3-methyl-4-nitrophenol	fenitrothion	15.1% (pH 9)	-	EPA 1995c
		15%	30 days	APVMA 1999
demethyl fenitrothion	fenitrothion	10.3% (pH 5 & 7)	-	EPA 1995c
		5.6% (pH 9)	-	EPA 1995c
M3	fenpyroximate	6.7%	30 days	PSD 1995e
1,3-dimethyl-5-phenoxypyrazole-4-carbonitrile	fenpyroximate	10.1%	30 days	PSD 1995e
RPA 20077	fipronil	53% (pH 9)	30 days	HSE 1999
RPA 200766	fipronil	52% (pH 9)	30 days	PSD 2004a
5-hydroxy-XDE-570	florasulam	14 - 32%	90 days	PMRA 2001c
fluazifop acid	fluazifop-P-butyl	major [g]	-	PMRA 1988
fluazifop acid	fluazifop-butyl	major [g]	-	PMRA 1988
compound V	fluazinam	major [g] (pH 7 & 9)	-	PMRA 2003j
MKH 6562 sulfonamide	flubcarbazone-sodium	3.9 - 4.2%	-	PMRA 2000c
RH-9985	fluoroglycofen-ethyl	48.1% (pH 5)	30 days	PSD 1992d
		64.7% (pH 7)	30 days	PSD 1992d
		21.3% (pH 9)	30 days	PSD 1992d
RH-5781	fluoroglycofen-ethyl	4% (pH 5)	30 days	PSD 1992d
		13.8% (pH 7)	30 days	PSD 1992d
		77.7% (pH 9)	30 days	PSD 1992d
M1	imazaquin	10% (pH 9)	30 days	PSD 1993h
N-carbamoyl-N-propargylglycine	imiprothrin	24.26% [h] (pH 7)	30 days	PMRA 2003l
		87.28% [h] (pH 9)	5 days	PMRA 2003l
1-propargylimidazolidine-2,4-dione	imiprothrin	1.81% [h] (pH 7)	30 days	PMRA 2003l
		4.26% [h] (pH 9)	5 days	PMRA 2003l
ioxynil	ioxynil octanoate	major [g]	-	EU 2004g
3-iodo-4-hydroxybenzonitrile	ioxynil octanoate	major [g]	-	EU 2004g
propargyl butyl carbamate	IPBC	12% (pH 7)	30 days	HSE 1994
		1% (pH 5)	30 days	HSE 1994
RP 35606	iprodione	11.4% (pH 5)	30 days	EU 2002n
		15% [b] (pH 7)	125 hours	EU 2002n
		11.9% (pH 5)	-	EPA 1998g
RP 30228	iprodione	46% (pH 7)	125 hours	EU 2002n
		92% [b] (pH 8)	2 hours	EU 2002n
		93.3% (pH 9)	-	EPA 1998g
RPA 202248	isoxaflutole	<10%	-	PMRA 2000e
RPA 203328	isoxaflutole	<10%	-	PMRA 2000e
RPA 205834	isoxaflutole	<10%	-	PMRA 2000e
malonic acid	kathon 886	<20%	-	HSE 1993
N-methyl malonamic acid	kathon 886	>20%	-	HSE 1993
malonamic acid	kathon 886	<20%	-	HSE 1993
ethylenethiourea	mancozeb	major [g] (pH 5)	-	EU 2005h
		major [g] (pH 7)	-	EU 2005h
ethyleneurea	mancozeb	trace [g] (pH 5)	-	EU 2005h
		trace [g] (pH 7)	-	EU 2005h
ethylenebisisothiocyanide sulfide	mancozeb	trace [g] (pH 5)	-	EU 2005h
		major [g] (pH 7)	-	EU 2005h
malathion monocarboxylic acids	malathion	1.8% (pH 5)	-	PSD 1995i
		23% (pH 7)	-	PSD 1995i
		40% (pH 9)	-	PSD 1995i
		15% (pH 8)	36 hours	PSD 1995i
ethyl hydrogen fumarate	malathion	0.6% (pH 5)	-	PSD 1995i
		19% (pH 7)	-	PSD 1995i
		36% (pH 9)	-	PSD 1995i
diethyl mercaptosuccinate	malathion	23% (pH 7)	-	PSD 1995i
		10% (pH 9)	-	PSD 1995i
malathion dicarboxylic acid	malathion	4% (pH 7)	-	PSD 1995i
		3% (pH 9)	-	PSD 1995i
diethyl fumarate and ethyl hydrogen fumarate combined	malathion	35% (pH 8)	36 hours	PSD 1995i
S-(1,2-di(carbethoxy)ethyl)-0-methyl hydrogen phosphorodithioate	malathion	8 - 10% (pH 4)	30 days	PSD 1995i
DIDT	mancozeb	44.5% (pH 7)	30 hours	PSD 2004b
		93.8% (pH 9)	0 hours	PSD 2004b
CGA-41638	metolachlor	3.63%	30 days	EPA 1995f
metolachlor oxanilic acid	metolachlor	3.54%	30 days	EPA 1995f
CGA-46129	metolachlor	3.42%	30 days	EPA 1995f
CGA-50720	metolachlor	3.2%	30 days	EPA 1995f
S-methyl-N-hydroxythioacetimidate	methomyl	41 - 44%	30 days	EPA 1998h
deaminated metribuzin	metribuzin	major [g]	-	EPA 1998i
IN-A4098	metsulfuron-methyl	~50% [b] (pH 5)	-	EU 2000c
IN-D5803	metsulfuron-methyl	25% [b]	-	EU 2000c

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Aqueous photolysis continued...				
methyl-2-(aminosulfonyl)benzoate	metsulfuron-methyl	26%	30 days	PSD 1991e
saccharin	metsulfuron-methyl	37%	30 days	PSD 1991e
		35% [b]	-	EU 2000c
ethylene bisisocyanate sulfide	nabam	major [g]	-	PSD 1994e
ethylenethiourea	nabam	major [g]	-	PSD 1994e
ASDM	nicosulfuron	53% (pH 5)	32 days	PSD 2000c
ADMP	nicosulfuron	65% (pH 5)	32 days	PSD 2000c
2-chloro-1-(3-hydroxy-4-nitophenoxy)-4-(trifluoromethyl) benzene	oxyfluorfen	1.3-1.7%	-	PSD 1996a
MHPC	phenmedipham	major [g]	-	EU 2004i
phorate sulfoxide	phorate	major [g]	-	PMRA 2003a
phorate sulfone	phorate	major [g]	-	PMRA 2003a
formaldehyde	phorate	major [g]	-	PMRA 2003a
phosmet oxon	phosmet	major [g]	-	PMRA 2004d
2-diethylamino-6-methylpyrimidin-4-ol	pirimiphos-methyl	main [g]	2 weeks	PSD 1991a
O,2-diethylamino-6-methylpyrimidin-4-yl-O,O-dimethyl phosphate	pirimiphos-methyl	significant [g]	2 weeks	PSD 1991a
CGA-171683	primisulfuron methyl	43.4%	-	PMRA 2001a
CGA-120844	primisulfuron methyl	46.8%	-	PMRA 2001a
RH24644	pronamide	<4%	-	EPA 1994f
RH24580	pronamide	<4%	-	EPA 1994f
RH25891	pronamide	<4%	-	EPA 1994f
Ro 17-3102	propaquizafop	major [g] (pH 7 and 9)	14 days	PSD 1994n
hydroxylamine derivative	propaquizafop	major [g] (pH 5)	14 days	PSD 1994n
CGA 300407	pymetrozine	77.1% (pH 5)	-	PMRA 2002
CGA 215525	pymetrozine	47.7% (pH 5)	-	PMRA 2002
CGA 249257	pymetrozine	2.6% (pH 5)	-	PMRA 2002
BF 500-5	pyraclostrobin	4%	-	PMRA 2003n
BF 500-6	pyraclostrobin	4%	-	PMRA 2003n
BF 500-7	pyraclostrobin	4%	-	PMRA 2003n
6-chloro-3-phenyl-4-hydroxy-pyridazine	pyridate	50%	66.7 hours	PMRA 1991a
Identified I	RH-287	31.4%	-	HSE 2004
Identified II	RH-287	5%	-	HSE 2004
Identified III	RH-287	1.9%	-	HSE 2004
IN-70941	rimsulfuron	17% [b]	-	PSD 1996f
IN-70942	rimsulfuron	84% [b]	-	PSD 1996f
IN-E9260	rimsulfuron	10% [b]	-	PSD 1996f
IN-J290	rimsulfuron	7% [b]	-	PSD 1996f
IN-T5831	rimsulfuron		-	PSD 1996f
sulphonamide	sulfosulfuron	major [g]	-	PMRA 1998
aminopyrimidine	sulfosulfuron	major [g]	-	PMRA 1998
anilino acid	tau-fluvalinate	58% (pH 9)	-	PSD 1997e
		18% [g] (pH 7)	-	PSD 1997e
dicarboxylic acid	tau-fluvalinate	15% (pH 9)	-	PSD 1997e
3-phenoxybenzoic acid	tau-fluvalinate	12% (pH 5)	-	PSD 1997e
3-phenoxybenzaldehyde	tau-fluvalinate	33% (pH 9)	-	PSD 1997e
		20% [g] (pH 7)	-	PSD 1997e
DP-2	tepraloxydim	68%	-	PMRA 2004b
DP-8	tepraloxydim	20%	-	PMRA 2004b
DP-6	tepraloxydim	2%	-	PMRA 2004b
DP-10	tepraloxydim	minor [g]	-	PMRA 2004b
GP	tepraloxydim	minor [g]	-	PMRA 2004b
FP	tepraloxydim	minor [g]	-	PMRA 2004b
cis-cyclopropanecarboxylic acid	tefluthrin	31 - 38% (pH 9)	-	PSD 1991h
2,3,5,6-tetrafluoro-4-methylbenzyl alcohol	tefluthrin	21 - 22% (pH 9)	-	PSD 1991h
hydroxyterbuthylazine	terbuthylazine	15.6% (pH 5)	50 days	PSD 1993a
2-ester-3-sulfonamide	thifensulfuron-methyl	64%	-	EU 2001g
2-ester-3-triuret	thifensulfuron-methyl	8 - 32%	-	EU 2001g
methyl 3-(aminosulphonyl)-2-thiophenecarboxylate	thifensulfuron-methyl	primary [g]	30 days	PSD 1991i
methomyl	thiodicarb	20% (pH 5)	30 days	EPA 1998k
		36% (pH 7)	30 days	EPA 1998k
		66% (pH 9)	1 days	EPA 1998k
carbendazim	thiophanate-methyl	primary [g]	-	EPA 2001c
AV-1951	thiophanate-methyl	primary [g]	-	EPA 2001c
DM-TM	tolclofos-methyl	major [g]	-	PSD 1993l
ph-CH3	tolclofos-methyl	major [g]	-	PSD 1993l
tralkoxydim metabolite 9	tralkoxydim	75.8 - 79% (pH 5)	28 days	PSD 1993m
		18.8% (pH 7)	14 days	PSD 1993m
2,3,5,6-tetrafluorobenzylalcohol	transfluthrin	81.9%	36 days	HSE 1997
triazamate metabolite II	triazamate	3% (pH 5)	30 days	PSD 1998d

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Aqueous photolysis continued...				
		13% (pH 7)	15 days	PSD 1998d
triazamate metabolite X	triazamate	6% (pH 5)	30 days	PSD 1998d
		70% (pH 7)	7 days	PSD 1998d
triazamate metabolite XI	triazamate	8% (pH 7)	15 days	PSD 1998d
		20% (pH 9)	30 days	PSD 1998d
triazmate polar metabolite 1	triazamate	83% (pH 9)	2 days	PSD 1998d
saccharin	tribenuron methyl	22 - 24% (pH 5 & 7)	32 days	PSD 1992h
sulphonamide A	tribenuron methyl	71 - 73% (pH 5 & 7)	32 days	PSD 1992h
acid sulphonamide A	tribenuron methyl	1% (pH 5 & 7)	32 days	PSD 1992h
triazine amine A	tribenuron methyl	94 - 96% (pH 5 & 7)	33 days	PSD 1992h
O-demethyl triazine amine A	tribenuron methyl	5 - 6% (pH 5 & 7)	33 days	PSD 1992h
triclopyr	triclopyr butoxyethyl ester	major [g]	-	EPA 1998l
CGA-321113	trifloxystrobin	major [g]	-	PMRA 2004h
methyl saccahrin	triflusulfuron-methyl	major [g]	-	PSD 1995r
		44 - 99%	-	PMRA 1999c
triazine amine B	triflusulfuron-methyl	major [g]	-	PSD 1995r
		43 - 98%	-	PMRA 1999c
trinexapac acid	trinexapac ethyl	<10% (pH 9)	-	PSD 1995s
		major [g] (pH 5 & 7)	-	PSD 1995s
		major [g] (pH 9)	-	PMRA 2001b
propane-1,2,3-tricarboxylic acid	trinexapac ethyl	>10% (pH 5)	-	PSD 1995s
pyrithione disulfide	zinc pyrithione	21.23% (pH 5)	30 days	HSE 2003b
		16.39% (pH 7)	30 days	HSE 2003b
		< 10% (pH 9)	30 days	HSE 2003b
pyrithione sulfinic acid	zinc pyrithione	<10% (pH 7)	30 days	HSE 2003b
		11.59% (pH 9)	30 days	HSE 2003b
carbonyl disulfide	ziram	81.6% (pH 5 & 7)	72 hours	PSD 1994c
		main [g] (pH 9)	-	PSD 1994c
RH-150721	zoxamide	37.6% (pH 4)	-	PMRA 2001d
RH-24549	zoxamide	30.9% (pH 4)	-	PMRA 2001d
RH-141288	zoxamide	50.2% (pH 9)	-	PMRA 2001d
RH-129151	zoxamide	24.5% (pH 7)	-	PMRA 2001d
soil photolysis				
3-phenoxybenzoic acid	alpha-cypermethrin	17% [b]	30 days	EU 2004b
3-phenoxybenzoic alcohol	alpha-cypermethrin	2.7% [b]	30 days	EU 2004b
1,2,4-triazole	amitrole	9.9% [b]	30 days	EPA 1998b
dihydroxy anilazine	anilazine	75%	20 days	PSD 1994b
sulphanilamide	asulam	27.6%	2 hours	EPA 1995a
deethylatrazine	atrazine	19.2%	3.5 days	Solomon et al. 1996
		7.9%	168 hours	APVMA 1997a
		13.3%	30 days	APVMA 1997a
deisopropylatrazine	atrazine	7.9%	7 days	Solomon et al. 1996
		17.4%	168 hours	APVMA 1997a
		11.9%	30 days	APVMA 1997a
diaminochloroatrazine	atrazine	6.8%	22 days	Solomon et al. 1996
		4.3%	168 hours	APVMA 1997a
reference compound 28	azoxystrobin	minor [g]	-	PMRA 2000a
reference compound 30	azoxystrobin	minor [g]	-	PMRA 2000a
LS 860551	bromuconazole	<2%	-	PSD 1996a
LS 860550	bromuconazole	<2%	-	PSD 1996a
RPA 401527	bromuconazole	<2%	-	PSD 1996a
LS 860364	bromuconazole	<2%	-	PSD 1996a
LS 830730	bromuconazole	<2%	-	PSD 1996a
DNTBA	butralin	<2.3%	-	PSD 1998a
tetrahydrophthalamide	captan	21.3%	5 days	EPA 1999a
cyclohex-4-ene-2-cyano-1-carboxylic acid	captan	9.4%	5 days	EPA 1999a
3-(3-chloro-p-tolyl)-1-methylurea	chlorotoluron	5.4%	3 days	EU 2005c
CCIM	cyazofamid	40% [g]	7 days	EU 2002e
CCBA	cyazofamid	37.6% [g]	21 days	EU 2002e
4-fluoro-3-phenoxybenzaldehyde	cyfluthrin	18% [b]	6 days	EU 2002c
compound Ia	*lambda*-cyhalothrin	<10%	-	EU 2001d
Q8761	cymoxanil	minor [g]	-	PMRA 2000b
aminooxacetic acid	cymoxanil	minor [g]	-	PMRA 2000b
JX915	cymoxanil	<11%	-	PMRA 2000b
W3595	cymoxanil	minor [g]	-	PMRA 2000b
U3204	cymoxanil	minor [g]	-	PMRA 2000b
T4226	cymoxanil	minor [g]	-	PMRA 2000b
KP533	cymoxanil	minor [g]	-	PMRA 2000b

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Aqueous photolysis continued...				
KQ960	cymoxanil	minor [g]	-	PMRA 2000b
R3273	cymoxanil	minor [g]	-	PMRA 2000b
1-(4-chlorophenyl)-2-(1H-1,2,4-triazol-1-yl)-ethanone	cyproconazole	5%	20 days	PSD 1991f
3-cyclopropyl-1-(1H-1,2,4-triazol-1-yl)butanone	cyproconazole	4%	20 days	PSD 1991f
MTP	dacthal	5.2%	-	EPA 1998d
decamethrinic acid	deltamethrin	36% [b]	30 days	EU 2002g
ethyl-m-hydroxyphenyl carbamate	desmedipham	7.4% [b]	488 hours	EPA 1996e
pyrimidinol	diazinon	56 - 62%	24 hours	PSD 1991b
		56%	24 hours	PSD 1991b
o,p'-dichlorobenzophenone	o,p'-dicofol	major [g]	-	EPA 1998f
p,p'-dichlorobenzophenone	p,p'-dicofol	major [g]	-	EPA 1998f
p-chlorophenyl urea	diflubenzuron	3% [b]	7 days	EPA 1997a
2,6-difluorobenzoic acid	diflubenzuron	12.9% [b]	10 days	EPA 1997a
SP1	diflubenzuron	0.6% [b]	10 days	EPA 1997a
PK1	diflubenzuron	0.1% [b]	16 days	EPA 1997a
O-desmethyldimethoate	dimethoate	major [g]	-	EPA 1999e
O,O-dimethylphosphorothioic acid	dimethoate	minor [g]	-	EPA 1999e
N'-(3,4-dichlorophenyl)-N-methylurea	diuron	major [g]	-	EPA 2003b
3,4-dichlorophenylurea	diuron	minor [g]	-	EPA 2003b
3,4-dichloroaniline	diuron	minor [g]	-	EPA 2003b
3,3',4,4'-tetrachlorobenzene	diuron	minor [g]	-	EPA 2003b
$CONH_2$-fen	esfenvalerate	48.4%	-	PSD 1992c
		25%	10 days	PSD 1992c
COOH-fen	esfenvalerate	2%	-	PSD 1992c
Cl-Vacid	esfenvalerate	4.5%	-	PSD 1992c
dec-fen	esfenvalerate	0.9%	-	PSD 1992c
s-trifluoromethyl-3-nitro-1,2-benzendiamine	ethalfluralin	>4.3%	-	PSD 1995l
2-(1-methyletenyl)-4-nitro-6-trifluoromethyl-1H-benzimidazole	ethalfluralin	>4.3%	-	PSD 1995l
2-methyl-7-nitro-5-trifluoromethyl-1H-benimidazole-3-oxide	ethalfluralin	>4.3%	-	PSD 1995l
ethylene	ethephon	major [g]	-	EPA 1995b
2-hydroxy ethyl phosphonic acid	ethephon	major [g]	-	EPA 1995b
IN-H3310	famoxadone	major [g]	-	PMRA 2003h
IN-MN467	famoxadone	major [g]	-	PMRA 2003h
IN-MN468	famoxadone	major [g]	-	PMRA 2003h
IN-KF015	famoxadone	major [g]	-	PMRA 2003h
IN-JS940	famoxadone	minor [g]	-	PMRA 2003h
HOE 83348	fenchlorazole-ethyl	8.9%	45 days	PSD 1990e
HOE 88988	fenchlorazole-ethyl	3.6%	16 days	PSD 1990e
HOE 88989	fenchlorazole-ethyl	1.6%	7 days	PSD 1990e
HOE 72829	fenchlorazole-ethyl	13%	3.7 days	PSD 1990e
HOE 87606	fenchlorazole-ethyl	4.6%	16 days	PSD 1990e
fenitrooxon	fenitrothion	3.6 - 9.4%	1 day	APVMA 1999
		1.6%	30 days	APVMA 1999
3-methyl-4-nitrophenol	fenitrothion	22 - 24%	7 days	APVMA 1999
		3.3%	14 days	APVMA 1999
desmethyl fenitrothion	fenitrothion	<1%	-	APVMA 1999
S-methyl fenitrothion	fenitrothion	<1%	-	APVMA 1999
carboxy-fenitrothion	fenitrothion	<1%	-	APVMA 1999
carboxy-fenitrooxon	fenitrothion	<1%	-	APVMA 1999
desmethyl fenitrooxon	fenitrothion	1.6%	30 days	APVMA 1999
α-carbomoyl-3-phenoxybenzyl-2,2,3,3-tetramethyl cyclopropane carboxylate	fenpropathrin	6 – 44%	5 – 7 days	PSD 1989a
		3 – 26% (dark)	14 days	PSD 1989a
MB 46513	fipronil	6.9%	30 days	PSD 2004a
RPA 104615	fipronil	7%	30 days	PSD 2004a
CGA 257 777	fludioxonil	8%	7 days	PSD 1995e
FBC 96912	fluquinconazole	7.5%	24.7 days	PSD 1999b
RH-5781	fluoroglycofen-ethyl	5.3%	13 days	PSD 1992d
RH-9985	fluoroglycofen-ethyl	19%	13 days	PSD 1992d
5-hydroxy-XDE-570	florasulam	major [g]	-	PMRA 2001c
8-fluoro-5-methoxy(1,2,4)triazolo(1,5c)-pyrimidine-2-sulphonamide	florasulam	major [g]	-	PMRA 2001c
vinyl fluoridetriazolo-florasulum	florasulam	minor [g]		PMRA 2001c
florasulam triazolo carboxylic acid	florasulam	minor [g]		PMRA 2001c
triazolo-florasulam	florasulam	minor [g]		PMRA 2001c
RE 54488	flurtamone	3.8%	-	PSD 2000a
RE 53285	flurtamone	0.5%	-	PSD 2000a
RE 54589	flurtamone	0.2%	-	PSD 2000a

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Aqueous photolysis continued...				
3-methyl phosphinico-proprionic acid	glufosinate ammonium	9.7%	16 days	PSD 1990f
3-cyclohexyl-6-(methylamino)-1-methyl-1,3,5-triazine-2,4(1H,3H)-dione	hexazinone	>10%	-	EPA 1994a
1-(6-chloro-pyridine-3-ylmethyl)-N-nitro-2-imino-imidazollidine-5-ol	imidacloprid	6.3 - 6.5%	7 - 15 days	PSD 1993i
1-(6-chloro-pyridine-3-ylmethyl)-N-nitroso-2-imino-imidazolidine	imidacloprid	<3%	7 - 15 days	PSD 1993i
6-chloro-nicotinic acid	imidacloprid	<3%	7 - 15 days	PSD 1993i
1-(6-chloro-pyridine-3-ylmethyl)-N-nitro-2-imino-2,3-dihydro-imidazole and 1-(6-chloro-pyridine-3-ylmethyl)-imazolidine-2-one combined	imidacloprid	<3%	7 - 15 days	PSD 1993i
AE 0002166	iodosulfuron-methyl	major [g]	-	PMRA 2004f
RP 25040 and LS70942 combined	iprodione	14% [b]	7 days	EU 2002n
RP 25040 and LS70942 combined	iprodione	13.75% [b]	7 days	EPA 1998g
3,5-dichloroaniline	iprodione	27.94% [b]	14 days	EPA 1998g
RP 30228	iprodione	7.72% [b]	0 days	EPA 1998g
RPA 202248	isoxaflutole	>70%	-	PMRA 2000e
RPA 203328	isoxaflutole	>30%	-	PMRA 2000e
kresoxim-methyl acid	kresoxim-methyl	7.4%	-	PSD 1997c
norlinuron	linuron	<8.4%	-	EPA 1995e
desmethyl linuron	linuron	<8.4%	-	EPA 1995e
3,4-dichloroaniline	linuron	<8.4%	-	EPA 1995e
RH-131154	methoxyfenozide	2%	14 days	PMRA 2004g
RH-117236	methoxyfenozide	1.5%	30 days	PMRA 2004g
metolachlor oxanilic acid	metolachlor	3.4%	21 days	EPA 1995f
CGA-37735	metolachlor	9%	21 days	EPA 1995f
CGA-41638	metolachlor	5.7%	21 days	EPA 1995f
CGA-40172	metolachlor	6.2%	21 days	EPA 1995f
CGA-37913	metolachlor	7.3%	21 days	EPA 1995f
acetonitrile	methomyl	40%	30 days	EPA 1998h
deaminated metribuzin	metribuzin	major [g]	-	EPA 1998i
pentylidene metribuzin	metribuzin	major [g]	-	EPA 1998i
hexylidene metribuzin	metribuzin	major [g]	-	EPA 1998i
saccharin	metsulfuron-methyl	10%	30 days	PSD 1991e
2-aminosulfonyl) benzoic acid	metsulfuron-methyl	8%	30 days	PSD 1991e
methyl-2-(aminosulfonyl)benzoate	metsulfuron-methyl	<1%	-	PSD 1991e
ASDM	nicosulfuron	23%	30 days	PSD 2000c
ADMP	nicosulfuron	3.5%	0 days	PSD 2000c
DMPU	nicosulfuron	2.6%	0 days	PSD 2000c
HMUD	nicosulfuron	1.1%	0 days	PSD 2000c
desmethyl norflurazon	norflurazon	6%	15 - 43 days	EPA 1996f
3,5-dinitro-4-amino-sulfanilamide	oryzalin	2.6%	-	EPA 1994d
2-ethyl-7-nitro-5-sulfonyl benzimidazole	oryzalin	3.2%	-	EPA 1994d
3,5-dinitro-N,N-dipropyl sulfanilic acid	oryzalin	4.6%	-	EPA 1994d
1,2,4-triazole	paclobutrazol	4.2%	33 days	PSD 1995j
3-aminophenol and methoxycarbonylaminophenol combined	phenmedipham	17.8% [b]	105 hours	EU 2004l
CGA-120844	primisulfuron methyl	43.9%	-	PMRA 2001a
CGA-171683	primisulfuron methyl	37.9%	-	PMRA 2001a
prochloraz-formylurea	prochloraz	12.4% [g]	-	Höllrigl-Rosta et al. 1999
prochloraz-urea	prochloraz	3.4% [g]	-	Höllrigl-Rosta et al. 1999
hydroxypropachlor	propachlor	4.3%	-	EPA 1998j
N-(1,1-dimethylacetonyl)-3,5-dichlorobenzamide	propyzamide	13%	28 days	EU 2003q
CGA 359009	pymetrozine	28.6 - 33.5%	-	PMRA 2002
CGA 300407	pymetrozine	7.6%	-	PMRA 2002
CGA 294849	pymetrozine	5.7%	-	PMRA 2002
BF 500-3	pyraclostrobin	minor [g]	-	PMRA 2003n
BF 500-6	pyraclostrobin	minor [g]	-	PMRA 2003n
BF 500-7	pyraclostrobin	minor [g]	-	PMRA 2003n
IN-70941	rimsulfuron	34.4 - 42.4%	27 days	PSD 1996f
IN-E9260	rimsulfuron	12.2%	27 days	PSD 1996f
IN-J290	rimsulfuron	12.7%	27 days	PSD 1996f
IN-T5831	rimsulfuron	9.4%	27 days	PSD 1996f
deisopropylatrazine	simazine	<6%	14 days	PSD 1992e
		7.5%	32 days	PSD 1992e
diaminochlorotriazine	simazine	<6%	14 days	PSD 1992e

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Aqueous photolysis continued...				
		9.7%	70 days	PSD 1992e
hydroxysimazine	simazine	<6%	14 days	PSD 1992e
		15 - 90%	32 weeks	PSD 1992e
deisopropyl deethylatrazine	simazine	<6%	14 days	PSD 1992e
sulphonamide	sulfosulfuron	23%	-	PMRA 1998
aminopyrimidine	sulfosulfuron	25%	-	PMRA 1998
anilino acid	tau-fluvalinate	<8%	-	PSD 1997e
dicarboxylic acid	tau-fluvalinate	10% [b]	9 days	PSD 1997e
3-phenoxybenzoic acid	tau-fluvalinate	<8%	-	PSD 1997e
3-phenoxybenzaldehyde	tau-fluvalinate	<8%	-	PSD 1997e
tau-fluvalinate amide	tau-fluvalinate	23% [b]	9 days	PSD 1997e
cyanohydrin	tau-fluvalinate	<8%	-	PSD 1997e
STJ 5706	tebuconazole	0.8 -1%	-	PSD 1993k
KFE 1224	tebuconazole	0.4 - 1.8%	-	PSD 1993k
HWG 3877	tebuconazole	1.1%	-	PSD 1993k
HWG 2685	tebuconazole	0.8 - 3.3%	-	PSD 1993k
SN 3678-7/A and SN 3678-7/B combined	tebuconazole	0.9 - 1.8%	-	PSD 1993k
1,2,4-triazole	tebuconazole	0.6 - 1%	-	PSD 1993k
CL 810 721	tebufenpyrad	<12%	-	PSD 1995o
CL 11 148	tebufenpyrad	<3%	-	PSD 1995o
CL 810 718	tebufenpyrad	<7%	-	PSD 1995o
cis-cyclopropanecarboxylic acid	tefluthrin	<2.6%	135 hours	PSD 1991h
trans-cyclopropanecarboxylic acid	tefluthrin	1.5%	135 hours	PSD 1991h
2,3,5,6-tetrafluoro-4-methylbenzyl alcohol	tefluthrin	1.6%	135 hours	PSD 1991h
DP-1	tepraloxydim	11%	-	PMRA 2004b
GP	tepraloxydim	22%	-	PMRA 2004b
FP	tepraloxydim	18%	-	PMRA 2004b
DP-2	tepraloxydim	5%	-	PMRA 2004b
DP-6	tepraloxydim	4%	-	PMRA 2004b
tetraconazole acid	tetraconazole	13%	60 days	PSD 1999c
		<10%	-	PSD 1999c
tetraconazole alcohol	tetraconazole	<5%	-	PSD 1999c
1,2,4-triazole	tetraconazole	<5%	-	PSD 1999c
tetraconazole difluoroacetic acid	tetraconazole	<10%	-	PSD 1999c
triazolylacetic acid	tetraconazole	<5%	-	PSD 1999c
2-ester-3-sulfonamide	thifensulfuron-methyl	20 - 24%	-	EU 2001g
		20%	30 hours	PSD 1991i
IN-A4098	thifensulfuron-methyl	9 - 32%	-	EU 2001g
		32%	30 hours	PSD 1991i
0-demethyl thifensulfuron methyl	thifensulfuron-methyl	2%	30 hours	PSD 1991i
		3%	30 hours	PSD 1991i
2-acid-3-sulfonamide	thifensulfuron-methyl	1%	30 hours	PSD 1991i
thiophene sulfonamide	thifensulfuron-methyl	0.3%	30 hours	PSD 1991i
thifensulfuron acid	thifensulfuron-methyl	2%	30 hours	PSD 1991i
triazine urea	thifensulfuron-methyl	2%	30 hours	PSD 1991i
methomyl	thiodicarb	22% [b]	-	PSD 1992f
		21%	30 days	EPA 1998k
methomyl oxime	thiodicarb	27% [b]	-	PSD 1992f
TM-SCH3	tolclofos-methyl	2.5% [b]	8 days	PSD 1993l
TMO	tolclofos-methyl	11 % [b]	2 days	PSD 1993l
DM-TM	tolclofos-methyl	1.0 % [b]	2 days	PSD 1993l
DM-TMO	tolclofos-methyl	8.4 % [b]	16 days	PSD 1993l
TM-CH2OH	tolclofos-methyl	5 % [b]	8 days	PSD 1993l
ph-CH3	tolclofos-methyl	12 % [b]	2 days	PSD 1993l
tralkoxydim metabolite 9	tralkoxydim	10.6 - 12.8%	11.5 days	PSD 1993m
tralkoxydim metabolite 10	tralkoxydim	5.8 - 6.7%	2.8 days	PSD 1993m
CGA 150829	triasulfuron	33%	-	PSD 1992g
G 28533 and CGA 188838 and CGA 195660 combined	triasulfuron	4.3%	-	PSD 1992g
sulphonamide A	tribenuron methyl	46.6% [b]	15 days	PSD 1992h
saccharin	tribenuron methyl	58.6% [b]	33 days	PSD 1992h
tribenuron methyl acid	tribenuron methyl	1.9% [b]	8 days	PSD 1992h
triazine amine A	tribenuron methyl	92.9% [b]	15 days	PSD 1992h
N-demethyl triazine amine A	tribenuron methyl	2.9% [b]	33 days	PSD 1992h
O-demethyl triazine amine A	tribenuron methyl	2.4% [b]	33 days	PSD 1992h
2,6-dinitro-N-propyl-4-trifluoromethylbenzenamine	trifluralin	6%	-	EPA 1996h
2-ethyl-7-nitro-5-trifluoromethyl-benimidazole-3-oxide	trifluralin	7.1%	-	EPA 1996h
N-demethyl triazine urea B	triflusulfuron-methyl	14%	-	PSD 1995r
		13.5%	-	PMRA 1999c
N-demethyl triflusulfuron-methyl	triflusulfuron-methyl	12%	-	PSD 1995r
		12.2%	-	PMRA 1999c
triazine amine B	triflusulfuron-methyl	12%	-	PSD 1995r
		11.8%	-	PMRA 1999c

Table A1. Pesticide transformation product formation in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	% of parent pesticide [b]	Time [c]	Reference
Aqueous photolysis continued...				
triazine urea B	triflusulfuron-methyl	7%	-	PSD 1995r
N-demethyl triazine amine B	triflusulfuron-methyl	7%	-	PSD 1995r
methyl saccharin	triflusulfuron-methyl	12%	-	PSD 1995r
		11.7%	-	PMRA 1999c
trinexapac acid	trinexapac ethyl	main [g]	-	PSD 1995s
		major [g]	-	PMRA 2001a
trinexapac metabolite 1 (CGA-163935)	trinexapac ethyl	main [g]	-	PSD 1995s
		major [g]	-	PMRA 2001a
RPA 406203	triticonazole	10.9% [b]	30 days	PSD 2000d
RPA 406341	triticonazole	<4%	-	PSD 2000d
RPA 406766	triticonazole	<4%	-	PSD 2000d
thriam	ziram	major [g]	-	PSD 1994c
RH-24549	zoxamide	22%	-	PMRA 2001d
RH-127450	zoxamide	11%	-	PMRA 2001d
dihydroxy product	zoxamide	6.73%	-	PMRA 2001d

a - pesticide identified in the reference as the source of the transformation product

b - peak percentage formation of transformation product during study

c - time to peak transformation product formation

d - soil and water system

e - soil before leaching in column leachate study

f - soil after leaching in column leachate study

g - no precise formation data provided

h - percentage of total recovery and not percentage of applied active

Table A2. The degradation of pesticide transformation products in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	Half-life / DT_{50}	Reference
Aqueous photolysis			
albendazole sulfoxide	albendazole	0.5 days (pH 7)	Weerasinghe et al. 1992
albendazole sulfone	albendazole	0.72 days (pH 7)	Weerasinghe et al. 1992
2-aminoalbendazole sulfone	albendazole	2.18 days (pH 7)	Weerasinghe et al. 1992
aldicarb sulfone	aldicarb	36 - 38 days	APVMA 2001
3-isopropyl-2,3-dioxo-5-oxocyclo-penteno[d]1H-2,1,3-thiadiazin-4(3H)-one 6-carbonic acid	bentazone	1.6 - 3.6 days	EU 2000a
3-carbamyl-2,4,5-trichlorobenzoic acid	chlorothalonil	53.7min (18°C)	EU 2005b
CCIM	cyazofamid	23.2 days	EU 2002e
HTID	cyazofamid	43.9 days	EU 2002e
CCTS	cyazofamid	2.2 days	EU 2002e
2,5-difluorobenzamide	flufenoxuron	stable (>38 days)	HSE 1995
flufenoxuron diphenyl amine	flufenoxuron	< 72 hours	HSE 1995
FBC 96912	fluquinconazole	2.3 hours (pH 4)	PSD 1999b
		1.4 hours (pH 9)	PSD 1999b
ethylenethiourea	metiram	358 days	EU 2005l
CL 153815	picolinafen	24.8 days (pH 5)	PMRA 2003m
		31.4 days (pH7)	PMRA 2003m
		22.6 days (pH 9)	PMRA 2003m
propylene urea	propineb	270 days - > 1year	EU 2003o
propylenethiourea	propineb	> 1 year	EU 2003o
6-chloro-3-phenyl-pyridazin-4-ol	pyridate	3.7 days (pH 5)	EU 2001e
		14.1 days (pH 7)	EU 2001e
		9.5 days (pH 9)	EU 2001e
		46 hours (pH 7)	PMRA 1991a
DP-1	tepraloxydim	14 days	PMRA 2004b
DP-2	tepraloxydim	6 days	PMRA 2004b
DP-6	tepraloxydim	7 days	PMRA 2004b
methomyl	thiodicarb	1 day	EPA 1998k
Surface water			
methamidophos	acephate	8.6 - 17.8 days	Sundaram 1993
ethyl-m-hydroxyphenyl carbamate	desmedipham	26 days	PSD 1993d
disulfoton sulfoxide	disulfoton	10.4 days (estuarine)	Lacorte et al. 1995
disulfoton sulfone	disulfoton	8.19 days (estuarine)	Lacorte et al. 1995
fenthion sulfoxide	fenthion	6.9 days (estuarine)	Lacorte et al. 1995
kresoxim-methyl acid	kresoxim-methyl	337 - 383 days	Roberts and Hutson 1999
BH518-5	quinmerac	stable	PSD 1998c
2,6-di-*tert*-butyl-4-methylphenyl carbamate	terbutol	47.1 months	Suzuki et al. 1998
2,6-di-*tert*-butyl-4-carboxyphenyl *N*-methylcarbamate	terbutol	63.6 months	Suzuki et al. 1998
2,6-di-*tert*-butyl-4-carboxyphenyl carbamate	terbutol	29.4 months	Suzuki et al. 1998
2,6-di-*tert*-butyl-4-methylphenol	terbutol	42 months	Suzuki et al. 1998
2,6-di-*tert*-butyl-4-carboxyphenol	terbutol	25 months	Suzuki et al. 1998
Hydrolysis (sterile)			
aldicarb sulfone	aldicarb	0.9 days (pH 9)	APVMA 2001
aldicarb sulfoxide	aldicarb	2.3 days (pH 9)	APVMA 2001
BTS 27271	amitraz	5 hours (alkaline)	EPA 1996a
		2280 days (acidic)	EPA 1996a
BTS 27919	amitraz	stable	EPA 1996a
3,5,-dibromo-4-hydroxybenzonitrile	bromoxynil	stable (pH 5, 7 and 9)	EPA 1998c
4-hydroxy-2,5,6-trichloroisophthalonitrile	chlorothalonil	stable (pH 5, 7 and 9)	PSD 2002
4-fluoro-3-phenoxybenzaldehyde	cyfluthrin	stable	EU 2002c
DCVA	cyfluthrin	> 1 year (pH 4, 7 and 9)	EU 2002c
diazoxon	diazinon	28.9 days	PSD 1991b
diclofop acid	diclofop-methyl	stable	EPA 2000b
RPA 200766	fipronil	stable (pH 9)	PSD 2004a
RH-9985	fluoroglycofen-ethyl	15.1 days (pH 9)	PSD 1992d
		5.3 days (pH 9)	PSD 1992d
FBC 96912	fluquinconazole	193 days (pH 9)	PSD 1999b
1,2,4-triazole	hexaconazole	stable (pH 5, 7 and 9)	PMRA 1995
RP 35606	iprodione	1.1 days (pH 7)	EU 2002n
		2.1 days (pH 8)	EU 2002n
RP 30228	iprodione	stable (pH 7)	EU 2002n
		1.8 days (pH 8)	EU 2002n
malathion monocarboxylic acids	malathion	26 days (pH 8)	PSD 1995l
malathion dicarboxylic acid	malathion	1 year (pH 9)	PSD 1995l
CL 153815	picolinafen	stable	PMRA 2003m
2,3,5,6-tetrachloroaniline	tecnazene	stable (pH 5, 7, 9)	PSD 1995p
methomyl	thiodicarb	stable (pH 5 and 7)	EPA 1998k
		30 days (pH 9)	EPA 1998k
		10 days (pH 9)	PSD 1992f
DMST	tolyfluanid	> 1 year (pH 4, 7, and 9)	PSD 1995q
triazamate metabolite X	triazamate	23.4 days (pH 7)	PSD 1998d
		15.6 hours (pH 9)	PSD 1998d

Table A2. The degradation of pesticide transformation products in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	Half-life / DT_{50}	Reference
Aerobic soil			
3-chloroaryl alcohol (mean of isomers)	1,3-dichloropropene	0.1 - 0.6 days	EFSA 2006a
3-chloroacrylic acid (mean of isomers)	1,3-dichloropropene	0.7 - 19.8 days	EFSA 2006a
trans-3-chloroallylalcohol	*trans*-1,3-dichloropropene	0.4 - 0.6 days	Dijk 1974
		0.8 - 1.4 days	Leistra et al. 1991
cis-3-chloroallylalcohol	cis-1,3-dichloropropene	1.2 - 1.8 days	Dijk 1974
		2.3 - 4.2 days	Leistra et al. 1991
2,4-D	2,4-DB	2.3 - 17.1 days	EU 2002a
methamidophos	acephate	3.5 - 9.3 days	Sundaram 1993
		<10 days	PSD 1995a
2-chloro-2',6'-diethylacetanilide	alachlor	2.4 days	Fava et al. 2000
2-hydroxy-2',6'-diethylacetanilide	alachlor	0.8 days	Fava et al. 2000
2,6-diethylaniline	alachlor	1.3 days	Fava et al. 2000
aldicarb sulfone	aldicarb	18 - 154 days	APVMA 2001
		84 - 1100 days (subsoil)	APVMA 2001
aldicarb sulfoxide	aldicarb	20 - 53 days	APVMA 2001
		84 - 410 days (subsoil)	APVMA 2001
BTS 27271	amitraz	67 - 82 days	EPA 1996a
		17 - 110 days (field)	EPA 1996a
BTS 27919	amitraz	61 -117 days	EPA 1996a
		70 - 150 days (field)	EPA 1996a
dihydroxy anilazine	anilazine	21 - 45 days	PSD 1994b
deethylatrazine	atrazine	26 days	Solomon et al. 1996
deisopropylatrazine	atrazine	17 days	Solomon et al. 1996
diaminochloroatrazine	atrazine	19 days	Solomon et al. 1996
hydroxyatrazine	atrazine	121 days	Solomon et al. 1996
benalaxyl M1	benalaxyl	49 - 90 days	EU 2004c
benalaxyl M2	benalaxyl	66 - 118 days	EU 2004c
carbofuran	benfuracarb	36 - 44 days	PSD 1998a
		30 - 34 days	PSD 1998a
		11 - 23 days	PSD 1998a
2-amino-N-isopropyl benzamide	bentazone	1 - 10 days (field)	EPA 2001a
3,5-dibromo-4-hydroxybenzamide	bromoxynil	0.47 - 5.2 days	EU 2004d
3,5-dibromo-4-hydroxybenzoic acid	bromoxynil	0.16 - 0.48 days	EU 2004d
3,5,-dibromo-4-hydroxybenzonitrile	bromoxynil octanoate	31 - 51 hours	EPA 1998c
tetrahydrophthalamide	captan	5.4 - 19.5 days	EPA 1999a
1-naphthol	carbaryl	14.93 days	Menon and Gopal 2003
N-phenyl-3-methyloxazoline-2,5-dione	carbetamide	21 - 23 days	Cantier et al. 1988
2-(phenylcarbamoyloxy)propionic acid	carbetamide	3.25 - 3.55 hours	Cantier et al. 1988
N-phenyl-2-hydroxypropionamide	carbetamide	25.4 - 27.9 days	Cantier et al. 1988
4-hydroxy-2,5,6-trichloroisophthalonitrile	chlorothalonil	6 - 43 days	PSD 2002
		130.6 days	EU 2005b
R417888	chlorothalonil	121.1 days	EU 2005b
3-carbamyl-2,4,5-trichlorobenzoic acid	chlorothalonil	103 days	EU 2005b
3,5,6-trichloro-2-pyridinol	chlorpyrifos / chlorpyrifos-methyl / triclopyr	42 - 117 days	Baskaran et al. 2003
		8 - 279 days	APVMA 2000b
		10 - 67 days	EU 2005d
		30 - 90 days	Tomlin 2000
		8 - 279 days	PMRA 1991b
3-methoxy-3,5,6-trichloropyridine	chlorpyrifos / triclopyr	33 - >72 days	Belfroid et al. 1996
		1 - 2 months	APVMA 2000b
		35 - >300 days	PMRA 1991b
chlorthal-dimethyl mono-acid	chlorthal-dimethyl	2.8 ± 0.1 days	Wettasinghe and Tinsley 1993
chlorthal-dimethyl di-acid	chlorthal-dimethyl	> 300 days	Wettasinghe and Tinsley 1993
clodinafop acid	clodinafop-propargyl	5 - 20 days	Tomlin 2000
		23 days	PSD 1995a
		9 - 13 days	PSD 1995a
		4.9 days	PSD 1995a
		5.1 days	PSD 1995a
cloquintocet acid	cloquintocet-mexyl	90 days	PSD 1995a
		5 -19 days	PSD 1995a
CCIM	cyazofamid	1.2 - 3.4 days	EU 2002e
		3.8 - 28.6 days	EU 2002e
CCIM-AM	cyazofamid	7.3 - 57 days	EU 2002e
		1 - 57 days	EU 2002e
CTCA	cyazofamid	236 - 395 days	EU 2002e
		17.7 - 395 days	EU 2002e
DCVA	cyfluthrin	12 - 62 days	EU 2002c
compound XV	*lambda*-cyhalothrin	7 - 16 days	EU 2001d
melamine	cyromazine	175 - 186 days (estimated)	PSD 1993c
		150 - 730 days (estimated)	PSD 1993c
2,4,6-triamino-1,3,5-triazine melamine	cyromazine	263 - 1086 days	Belfroid et al. 1996
MTP	dacthal	2.8 days	EPA 1998d
methyl isothiocyanate	dazomet / metam-sodium	10 days	Belfroid et al. 1996

Table A2. The degradation of pesticide transformation products in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	Half-life / DT_{50}	Reference
Aerobic soil continued...			
		4 - 5 days	Roberts and Hutson 1999
decamethrinic acid	deltamethrin	0.7 - 9.1 days (25°C)	EU 2002g
ethyl-m-hydroxyphenyl carbamate	desmedipham	21 days (15°C)	PSD 1993d
		9 days (25°C)	PSD 1993d
		27 days (15°C)	PSD 1993d
		21 days (25°C)	PSD 1993d
diazoxon	diazinon	17 hours	PSD 1991b
3,6-dichlorosalicylic acid	dicamba	> 40 days	Pearson et al. 1996
dicolfop-methyl and diclofop acid combined	diclofop-methyl	21 - 93 days	PSD 1991c
		10 - 38 days	PSD 1991c
		21 - 52 days	PSD 1991c
diclofop acid	diclofop-methyl	10 - 30 days	PSD 1991c
		6 - 38 days	PSD 1991c
		63 days	PSD 1991c
		26 - 28.4 days	PSD 1991c
omethoate	dimethoate	17 days	Belfroid et al. 1996
disulfoton sulfone	disulfoton	166 days	EPA 2002a
disulfoton sulfoxide	disulfoton	166 days	EPA 2002a
N'-(3,4-dichlorophenyl)-1-methylurea	diuron	217 - 1733 days	EPA 2003b
dipropylamine	EPTC	7 days	EPA 1999c
EPTC sulfoxide	EPTC	13 - 14 days	EPA 1999c
IN-KZ007	famoxadone	1.5 - 10.3 days	PMRA 2003h
IN-KF015	famoxadone	1.2 days	PMRA 2003h
IN-JS940	famoxadone	6 -23 hours	PMRA 2003h
fenamiphos sulfoxide	fenamiphos	62 days	PSD 1990b
fenamiphos sulfone	fenamiphos	29 days	PSD 1990b
3-methyl-4-nitrophenol	fenitrothion	6 - 13 days	PMRA 2003g
		12 days	EPA 1995c
fenoxaprop-ethyl acid	fenoxaprop-ethyl	5 - 14 days	PSD 1990c
5-hydroxy-XDE-570	florasulam	10 - 57 days	PMRA 2001c
fluazifop	fluazifop-p-butyl	3 - 16 weeks	PMRA 1988
fluazifop	fluazifop-butyl	3 - 16 weeks	PMRA 1988
MKH 6562 sulphonamide	flubcarbazone-sodium	> 400 days	PMRA 2000c
RH-5781	fluoroglycofen-ethyl	14 - 128 days	PSD 1992d
FBC 96912	fluquinconazole	448 days	PSD 1999a
4-amino-3,5-dichloro-6-fluoro-2-pyridinol	fluroxypyr	21 - 53 days	EU 1999
4-amino-3,5-dichloro-6-fluoromethoxypyridine	fluroxypyr	20 - 429 days	EU 1999
fluroxypyr	fluroxpyr-meptyl	< 7 days	Roberts 1998
phthalimide	folpet	17.2 days	PSD 1997a
AE F153745	formasulfuron	< 1 day	PMRA 2003k
dimethoate	formothion	7 - 40 days	Belfroid et al. 1996
formothioic acid	formothion	9 - 10 days	Belfroid et al. 1996
HOE 35950	glufosinate ammonium	4 - 42 days	PSD 1990f
3-methyl phosphinico-proprionic acid	glufosinate ammonium	165 days	PSD 1990f
		7 - 14 days	PSD 1990f
		13 - 22 days	PSD 1990f
aminomethylphosphonic acid	glyphosate and glyphosate trimesium	18 - 875 days [b]	EU 2002l
		127.8 - 140.6 days	EPA 1993b
		119 - 958 days	EPA 1993b
1,2,4-triazole	hexaconazole	14 weeks	PMRA 1995
metsulfuron-methyl	iodosulfuron-methyl	20 - 99 days	PMRA 2004f
AE F161778	iodosulfuron-methyl	9.4 - 21.1 days	PMRA 2004f
AE F059411	iodosulfuron-methyl	119 - 269 days	PMRA 2004f
3,5-di-iodo-4-hydroxybenzamide	ioxynil and ioxynil octanoate	3.7 - 7.7 days	EU 2004g
3,5-di-iodo-4-hydroxybenzoic acid	ioxynil	<2 days	EU 2004g
ioxynil	ioxynil octanoate	1.5 - 2.5 days	EU 2004g
propargyl butyl carbamate	IPBC	4.3 days	HSE 1994
		4.31 days	PSD 1987
RP 30228	iprodione	215 - 319 days	EU 2002n
desmethylisoproturon	isoproturon	22 - 65 days	EU 2002p
RPA 202248	isoxaflutole	24 - 96 days	PMRA 2000e
		11 - 26 days (field)	PMRA 2000e
RPA 203328	isoxaflutole	289 - 977 days	PMRA 2000e
		9 - 73 days (field)	PMRA 2000e
kresoxim-methyl acid	kresoxim-methyl	38 -131 days	Roberts and Hutson 1999
		38 days	PSD 1997c
		131 days	PSD 1997c
		57 days	PSD 1997c
		58.8 - 131 days	PMRA 2003c
kresoxim-methyl and kresoxim-methyl acid combined	kresoxim-methyl	20 - 425 days	PSD 1997c
		18 - 125 days (field)	PSD 1997c

Table A2. The degradation of pesticide transformation products in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	Half-life / DT_{50}	Reference
		12 - 52 days (field)	PMRA 2003c
Aerobic soil continued...			
490M5	kresoxim-methyl	<2 - 13 days (field)	PMRA 2003c
		4 -18 days (field)	PMRA 2003c
MCPA acid	MCPA	24 days	PSD 1988b
MCPA	MCPB	24 days	EU 2005k
ethylenethiourea	mancozeb/maneb/metiram	1.3 - 11 hours	PSD 2004b
		2.5 days	Calumpang et al. 1993
		2 hours	EU 2005h
		2 hours - 1 day	EU 2005l
		0.2 - 2 days	EU 2005l
ethyleneurea	mancozeb/maneb	4.8 days	Calumpang et al. 1993
		6.2 days	EU 2005h
		4.8 - 7.6 days	EU 2005l
ethylenebisisothiocyanide sulphide	maneb/metiram	0.09 - 0.15 days	EU 2005l
		0.09 - 0.8 days	EU 2005l
TDIT	metiram	0.3 - 0.9 days	EU 2005l
carbimid	metiram	0.009 - 0.9 days	EU 2005l
HOE 113225	mefenpyr-diethyl	9 days	PSD 1999a
HOE 094270	mefenpyr-diethyl	135 days	PSD 1999a
2-ethyl-6-methylaniline	metolachlor	1.7 days	Fava et al. 2000
IN-A4098	metsulfuron-methyl	210 days	EU 2000c
IN-D5803	metsulfuron-methyl	<< 1 month	EU 2000c
saccharin	metsulfuron-methyl	51 - 156 days [b]	EU 2000c
ADMP	nicosulfuron	2 - 7 days	PSD 2000c
ASDM	nicosulfuron	95 - 113 days	PSD 2000c
AUSN	nicosulfuron	53 - 91 days	PSD 2000c
UCSN	nicosulfuron	128 days	PSD 2000c
paraoxon	parathion	4 hours [a]	Saffih-Hdadi et al. 2003
phorate sulfoxide	phorate	65 - 137 days	PMRA 2003a
phorate sulfone	phorate	65 - 137 days	PMRA 2003a
CL 153815	picolinafen	30 - 77 days	PMRA 2003m
1,2,4-triazole	propiconazole	2 - 12 days	EU 2003n
CGA 118 245	propiconazole	<1 day	EU 2003n
propylene urea	propineb	4 - 93 days	EU 2003o
propylenethiourea	propineb	1.5 - 2.6 days	EU 2003o
2-(3,5-dichlorophenyl)-4,4-dimethyl-5-methyleneoxazoline	propyzamide	25.8 - 37.9 days	EU 2003q
N-(1,1-dimethylacetonyl)-3,5-dichlorobenzamide	propyzamide	12.4 - 16.7 days	EU 2003q
6-chloro-3-phenyl-pyridazin-4-ol	pyridate	< 14 - 60 days [b]	EU 2001e
		< 33 days (field)	PMRA 1991a
BH518-2	quinmerac	17 - 1080 days	PSD 1998c
BH518-5	quinmerac	4 - 3850 days	PSD 1998c
anilino acid	tau-fluvalinate	5.7 days	PSD 1997e
		7.1 days	PSD 1997e
DP-1	tepraloxydim	28 days (field)	PMRA 2004b
DP-2	tepraloxydim	198 - 235 days (field)	PMRA 2004b
2,6-di-*tert*-butyl-4-methylphenyl carbamate	terbutol	291 days	Suzuki et al. 2001
2,6-di-*tert*-butyl-4-carboxyphenyl *N*-methylcarbamate	terbutol	173 days	Suzuki et al. 2001
2,6-di-*tert*-butyl-4-carboxyphenyl carbamate	terbutol	184 days	Suzuki et al. 2001
thifensulfuron acid	thifensulfuron-methyl	2.2 - >365 days	EU 2001g
		20 - 157 days	EU 2001g
O-desmethyl thifensulfuron-methyl	thifensulfuron-methyl	10.8 - 15.3 days	EU 2001g
		< 2.9 days	EU 2001g
thiophene sulfonimide	thifensulfuron-methyl	9.6 - 96.6 days	EU 2001g
		41 - 69 days	EU 2001g
IN-A4098	thifensulfuron-methyl	176 days	EU 2001g
		22 - 43 days	EU 2001g
2-ester-3-sulfonamide	thifensulfuron-methyl	6 - 7 days	EU 2001g
methomyl	thiodicarb	45 days	EPA 1998k
carbendazim	thiophanate-methyl	320 days	EPA 2001c
		15 - 94 days [b]	EPA 2001c
		39.8 days	EU 2005m
DMST	tolyfluanid	0.24 - 8 days (estimated)	PSD 1995q
tridimenol	triadimefon	> 2 years	Bromilow et al. 1999
CGA 150829	triasulfuron	159 - 289 days	EU 2000d
triazamate metabolite II	triazamate	1.7 - 5.4 days	PSD 1998d
		3.2 - 70 days	PSD 1998d
triazine amine A	tribenuron methyl	240 days	PSD 1991g
		110 - 220 days	EFSA 2004
		38 - 144 days (field)	EFSA 2004
IN-A4098	tribenuron-methyl	22 - 39 days	EFSA 2004
saccahrin	tribenuron-methyl	230 days	EFSA 2004
2-butoxyethanol	triclopyr butoxyethyl	0.058 - 0.375 days	EPA 1998l

Table A2. The degradation of pesticide transformation products in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	Half-life / DT_{50}	Reference
CGA-321113	ester trifloxystrobin	250 - 350 days	PMRA 2004h
Aerobic soil continued...			
		215 - 350 days (field)	PMRA 2004h
trinexapac acid	trinexapac ethyl	1.1 - 21.4 days	PSD 1995s
		16 - 18 days	PSD 1995s
		5.1 days (field)	PSD 1995s
		43 days (field)	PSD 1995s
		5.1 - 31.5 days (field)	PMRA 2001b
RPA 406341	triticonazole	130 days (field)	PSD 2000d
		165 - 330 days	PMRA 2004c
RPA 407922	triticonazole	0.5 - 1.1 days	PMRA 2004c
Anaerobic soil			
aldicarb sulfone	aldicarb	5.6 - 131 days (subsoil)	APVMA 2001
aldicarb sulfoxide	aldicarb	2 - 27 days (subsoil)	APVMA 2001
CCIM	cyazofamid	4.7 days	EU 2002e
CCIM-AM	cyazofamid	35.4 days	EU 2002e
CTCA	cyazofamid	slow	EU 2002e
		17.7 - 395 days	EU 2002e
diclofop acid	diclofop-methyl	> 150 days	PSD 1991c
		>60 days	EPA 2000b
fenoxaprop-ethyl acid	fenoxaprop-ethyl	30 days	PSD 1990c
6-chloro-3-phenyl-pyridazin-4-ol	pyridate	stable	EU 2001e
methomyl	thiodicarb	<7 - 14 days	EPA 1998k
triazamate metabolite II	triazamate	15.3 - 137 days	PSD 1998d
CGA-321113	trifloxystrobin	1733 days	PMRA 2004h
Water/sediment systems			
BTS 27271	amitraz	6 - 7 days	EPA 1996a
BTS 27919	amitraz	9 -21 days	EPA 1996a
bromoxynil	bromoxynil octanoate	9.6 - 15.9 days (whole system)	EU 2004d
		4 -17 days (whole system)	EU 2004d
		3 - 15 days (water)	EU 2004d
		9.6 - 16 days (water)	EU 2004d
clodinafop acid	clodinafop-propargyl	56 days (sediment)	PSD 1995a
cloquintocet acid	cloquintocet-mexyl	46 days (sediment)	PSD 1995a
CCIM	cyazofamid	22.8 - 26.4 days	EU 2002e
4-fluoro-3-phenoxybenzoic acid	cyfluthrin	~10 days (water)	EU 2002c
3-phenoxybenzoic acid	*alpha*-cypermethrin	2.1 - 3 days	EU 2004b
dimethylcyclopropane carboxylic acid	*alpha*-cypermethrin	13.9 - 36.8 days	EU 2004b
ethyl-m-hydroxyphenyl carbamate	desmedipham	25 days (whole system)	PSD 1993d
		43 days (sediment)	PSD 1993d
		26 days (water)	PSD 1993d
		211.9 days (anaerobic)	EPA 1996e
diclofop acid	diclofop-methyl	27 days	PSD 1991c
		105 days (anaerobic)	PSD 1991c
4-(2,4-dichlorophenoxy)phenol	diclofop-methyl	32 days	PSD 1991c
5-hydroxy-*XDE*-570	florasulam	169 days (aerobic)	PMRA 2001c
1,2,4-triazole	fluquinconazole	42 - 190 days (water)	PSD 1999b
FBC 96912	fluquinconazole	73 - 89 days (water)	PSD 1999b
fluroxypyr	fluroxpyr-meptyl	< 7 days	Roberts 1998
metsulfuron-methyl	iodosulfuron-methyl	34.4 - 55.2 days (whole system)	PMRA 2004f
		291 days (anaerobic, whole system)	PMRA 2004f
AE F161778	iodosulfuron-methyl	2.9 - 21.3 days (whole system)	PMRA 2004f
AE F059411	iodosulfuron-methyl	87.6 days (whole system)	PMRA 2004f
AE 0014966	iodosulfuron-methyl	5.8 - 20.8 days (whole system)	PMRA 2004f
propargyl butyl carbamate	IPBC	11.5 days (anaerobic)	HSE 1994
RPA 202248	isoxaflutole	255 - 703 days (whole system)	PMRA 2000e
		66 - 89 days (water)	PMRA 2000e
		316 days (water, anaerobic)	PMRA 2000e
RPA 205834	isoxaflutole	52 - 97 days (whole system)	PMRA 2000e
		36 days (water)	PMRA 2000e
		48 days (water, anaerobic)	PMRA 2000e
		236 days (sediment, anaerobic)	PMRA 2000e
		131 days (whole system, anaerobic)	PMRA 2000e

Table A2. The degradation of pesticide transformation products in environmental systems (Chapter 2)

Transformation product	Parent pesticide [a]	Half-life / DT_{50}	Reference
kresoxim-methyl acid	kresoxim-methyl	464 - 473 days (whole system)	PSD 1997c
		337 - 383 days (water)	PSD 1997c
		>>92 - 462 days	PMRA 2003c
Water/sediment systems continued...			
		98 -130 days (anaerobic)	PMRA 2003c
ethylenethiourea	mancozeb/maneb / metiram	4 - 6.3 days (water)	PSD 2004b
		2 - 6.4 days (sediment)	PSD 2004b
		4 - 11.1 days (water)	EU 2005h; EU 2005i
		6.7 - 11.1 days (whole system)	EU 2005h
		7.4 - 7.6 days (whole system)	EU 2005i
		5.4 days (water)	EU 2005l
		5.9 - 6.5 days (whole system)	EU 2005l
ethyleneurea	maneb	< 20 days (water)	EU 2005i
		< 20 days (whole system)	EU 2005i
ethylenebisisothiocyanide sulfide	maneb	< 1 day (water)	EU 2005i
		< 1 day (whole system)	EU 2005i
MCPA acid	MCPA	> 30 days	PSD 1988b
HOE 113225	mefenpyr-diethyl	31 days (water)	PSD 1999a
		24 - 42 days (sediment)	PSD 1999a
		33 - 67 days (whole system)	PSD 1999a
HOE 094270	mefenpyr-diethyl	44 days (water)	PSD 1999a
		56 days (sediment)	PSD 1999a
		44 days (whole system)	PSD 1999a
HOE 109453	mefenpyr-diethyl	41 days (sediment)	PSD 1999a
phorate sulfoxide	phorate	9 days	PMRA 2003a
phorate sulfone	phorate	21 days	PMRA 2003a
CL 153815	picolinafen	45.3 - 70.1 days (water)	PMRA 2003m
		10.9 - 24.4 days (water)	PMRA 2003m
		197 days (anaerobic, water)	PMRA 2003m
		645 days (anaerobic, sediment)	PMRA 2003m
propylene urea	propineb	<30 days (whole system)	EU 2003o
propylenethiourea	propineb	4 days (water)	EU 2003o
2,3,5,6-tetrachloroaniline	tecnazene	83 - 105 days	PSD 1995p
DP-1	tepraloxydim	12.4 - 43.2 days	PMRA 2004b
thifensulfuron acid	thifensulfuron-methyl	66 -109 days (water)	EU 2001g
O-desmethyl thifensulfuron acid	thifensulfuron-methyl	27 - 51 days (water)	EU 2001g
IN-A4098	thifensulfuron-methyl	49 - 71 days (water)	EU 2001g
carbendazim	thiophanate-methyl	61 days	EPA 2001c
		743 days (anaerobic)	EPA 2001c
DMST	tolyfluanid	41 - 74 days	PSD 1995q
triazine amine A	tribenuron methyl	105 days (anaerobic)	PSD 1992h
		78 days (whole system)	EFSA 2004
saccharin	tribenuron-methyl	5.5 days (water)	EFSA 2004
triclopyr	triclopyr butoxyethyl ester	1300 days (anaerobic)	EPA 1998l
2-butoxyacetic acid	triclopyr butoxyethyl ester	1 day	EPA 1998l
		73.3 days (anaerobic)	EPA 1998l
2-butoxyethanol	triclopyr butoxyethyl ester	1.4 days (anaerobic)	EPA 1998l
		0.6 - 3.4 days	EPA 1998l
CGA-321113	trifloxystrobin	289 days	PMRA 2004h

a - DT_{100}

b - Soil DT_{50} during field study

Table A3. The adsorption of pesticide transformation products in environmental systems (Chapter 2)

Transformation product	Parent pesticide	K_d			K_{oc}			K_f			K_{foc}			1/n			Reference(s)
		range	mean	n	range	mean	n	range	mean	n	range	mean	n	range	mean	n	
(EZ)-3-chloroacrylic acid	1,3-dichloropropene				<1-17.5	3.8											EFSA 2006a
(EZ)-3-chloroallyl alcohol	1,3-dichloropropene				5.3-11.9	9.4											EFSA 2006a
2,4-dichlorophenol	2,4-D	2.6-5.02	3.7	4		108[a]											Haberhauer et al. 2000; Fava et al. 2005
2,4-D[e]	2,4-DB	0.22-3.08	1.6	5	31-74	47.8	5										EU 2002a
R1	acequinocyl				1175-22813	95264.3	3										PMRA 2007a
IC-0	acetamiprid							0.57-1.03	0.75	5	70-258	122	5	0.89-1.01	0.95	5	EU 2004a
IM-1-2	acetamiprid							0.16-3.6	1.12	4	19-95	54	4	0.86-0.94	0.9	4	EU 2004a
IM-1-4	acetamiprid							2.16-5.79	3.22	4	132-223	171	4	0.71-0.82	0.82	4	EU 2004a
IM-1-5	acetamiprid				453-563	508	2										EU 2004a
CGA 210007	acibenzolar-s-methyl							0.3-2.3	1	6	40-312	138.3	6	0.76-0.87	0.83	6	EU 2002b
2,6-diethylaniline	alachlor					357[a]											Fava et al. 2000
2-chloro-2',6'-diethylacetanilide	alachlor					148[a]											Fava et al. 2000
2-hydroxy-2',6'-diethylacetanilide	alachlor					45[a]											Fava et al. 2000
alachlor ethane sulfonic acid	alachlor				15-182	98.5	2										APVMA 2001; Aga and Thurman 2001
aldicarb sulfone	aldicarb										11-32	17.5	4		1.11		APVMA 2001
												29[d]					APVMA 2001
aldicarb sulfoxide	aldicarb										13.3-74.3	31.6	4		1.3		APVMA 2001
												47.9[d]					APVMA 2001
3-phenoxybenzoic acid	alpha-cypermethrin					73[c]											EU 2004b
2-amino-4,6-dimethoxypyrimidine	amidosulfuron					29[a]		1.05-81.3	14.8	8	89-11289	1860.6	8	0.52-0.86	0.67	8	PSD 1994a
4,6-dihydroxypyrimidin-2-yl-urea	amidosulfuron					0.4[a]											PSD 1994a
HOE 101630[e]	amidosulfuron					3[a]		0.08-0.83	0.51	5	24-63	43.8	5	0.45-0.6	0.53	5	PSD 1994a
								0.13-1.04	0.44	3	11.6-33.1	19.1	3	0.89-0.97	0.93	3	EFSA 2007a
dihydroxy anilazine	anilazine							0.92-7.39	3.81	4	144-437	350.8	4	0.68-0.88	0.78	4	PSD 1994b
deethylatrazine	atrazine	0.06-6.5	1.05	11	10-67	38.9	18		0.89								Brouwer et al. 1990; PSD 1992a; Mills and Thurman 1994; Solomon et al. 1996; APVMA 1997a; Steinheimer and Scoggin 2001; EPA 2003a

Table A3. The adsorption of pesticide transformation products in environmental systems (Chapter 2)

Transformation product	Parent pesticide	K_d range	K_d mean	K_d n	K_{oc} range	K_{oc} mean	K_{oc} n	K_f range	K_f mean	K_f n	K_{foc} range	K_{foc} mean	K_{foc} n	1/n range	1/n mean	1/n n	Reference(s)
		0.94-2.54			99-201												Oliver et al. 2005
deisopropylatrazine	atrazine & simazine	0.16-8.6	1.71	9		58.6	17		<3								Brouwer et al. 1990; PSD 1992a; PSD 1992e; Mills and Thurman 1994; Solomon et al. 1996; APVMA 1997a; Steinheimer and Scoggin 2001; EPA 2003a
					41-79												APVMA 1997a
		0.59-2.01			60-157												Oliver et al. 2005
diaminochlorotriazine	atrazine & simazine	0.16-1.56	0.68	4	31-76	55	4		<3								PSD 1992e; Solomon et al. 1996; APVMA 1997a; EPA 2003a
		0.1-0.8			11-59												PSD 1992a
hydroxyatrazine	atrazine	0.16-389	47.73	13	103-13797	1677.6	12										Brouwer et al. 1990; PSD 1992a; Solomon et al. 1996; APVMA 1997a; EPA 2003a
					177-1028												EPA 2003a
reference compound 2	azoxystrobin				33-770	328.7	6										PMRA 2000a; PMRA 2007f
reference compound 28	azoxystrobin				90-810	285	6										PMRA 2000a; PMRA 2007f
reference compound 30	azoxystrobin				40-250	106	6										PMRA 2000a; PMRA 2007f
benalaxyl M1	benalaxyl	7.03-21.7		3	151-455	375.6	3	8.4-18.1		4							EU 2004c
benalaxyl M2	benalaxyl	1.22-12.28		3	80-756	321	3	1.2-12.28		3							EU 2004c
carbofuran	benfuracarb	0.3-0.55	0.43	4	17-28	22	4										EFSA 2006b
2-amino-N-isopropyl benzamide	bentazone				30-97												Gaston et al. 1996
N-methyl bentazone	bentazone				250-350	300	2										Gaston et al. 1996
M-1	benthiavalicarb							1.3-11.2	7.1	3	237.2-422.3	299.9	3	0.76-0.78		3	EFSA 2007b
M-3	benthiavalicarb							1.9-5.5	3.9	3	116.4-241	168.7	3	0.79-0.82		3	EFSA 2007b
M-4	benthiavalicarb							3.3-10.4	6.9	3	221.4-407.8	296.8	3	0.82-0.91		3	EFSA 2007b
M-5	benthiavalicarb							4.6-23.2	16.6	3	494.4-787.3	618.1	3	0.73-0.79		3	EFSA 2007b
DCVA[a]	beta-cyfluthrin				14-356	133.7	3										EU 2002c

Table A3. The adsorption of pesticide transformation products in environmental systems (Chapter 2)

Transformation product	Parent pesticide	K_d range	K_d mean	K_d n	K_{oc} range	K_{oc} mean	K_{oc} n	K_f range	K_f mean	K_f n	K_{foc} range	K_{foc} mean	K_{foc} n	1/n range	1/n mean	1/n n	Reference(s)
D1989	bifenazate				3725-3962	3864	3	77-84	81.3	3							EU 2005a
						6189[d]			246[d]								EU 2005a
D3598	bifenazate					8710[b]											EU 2005a
3,5-dibromo-4-hydroxybenzamide	bromoxynil							0.5-9.2		4	32-330		4	0.67-0.87		4	EU 2004d
3,5-dibromo-4-hydroxybenzoic acid	bromoxynil							3.1-10.5		3	284-639		3	0.72-0.76		3	EU 2004d
THPAM	captan				3.8-110	45.2	6										EFSA 2006c
THPI	captan										5.7-11	8.1	5	0.83-1	0.91	5	EFSA 2006c
												2.2					EPA 1999a
1-naphthol	carbaryl					245[a]											EFSA 2006d
F8426-benzoic acid	carfentrazone-ethyl							0.12-0.58	0.24	5	5-41	17.2	5	0.77-1.01	0.88	5	EU 2003a
F8426-chloropropionic acid	carfentrazone-ethyl							0.11-0.59	0.35	5	7.4-46.4	23.4	5	0.86-0.91	0.89	5	EU 2003a
F8426-cinnamic acid[e]	carfentrazone-ethyl							0.35-7.77	2.85	5	44-333	141.8	5	1.1-1.14	1.11	5	EU 2003a
F8426-propionic acid[e]	carfentrazone-ethyl							0.19-6.07	2.05	5	27-260	98.2	5	1.13-1.34	1.21	5	EU 2003a
methyl triazole	carfentrazone-ethyl				27-94												EU 2003a
sulfonate	carfentrazone-ethyl				15-119												EU 2003a
metabolite B	chloridazon							0.34-0.71	0.48	4	29-74	49.5	4	0.79-0.87	0.83	4	EFSA 2007c
metabolite B1	chloridazon							0.4-7.34	1.67	6	27-136	91.8	6	0.79-0.92	0.87	6	EFSA 2007c
3-carbamyl-2,4,5-trichlorobenzoic acid	chlorothalonil				74-169												PSD 2002; EU 2005b
4-hydroxy-2,5,6-trichloroisophthalonitrile	chlorothalonil				95-1100	467.5	18										PSD 2002; EU 2005b
R417888	chlorothalonil				6-17	10	6										EU 2005b
3,5,6-trichloro-2-methoxypyridine	chlorpyrifos & chlorpyrifos-methyl	7.7-39.4	20.1	5	565-1308	888	5										EU 2005d; EU 2005e
3,5,6-trichloro-2-pyridinol	chlorpyrifos, triclopyr & chlorpyrifos-methyl	0.45-2.86			70-159												EPA 1998l; EPA 1999d; APVMA 2000b; Baskaran et al. 2003; EU 2005d
					27-389	165	29										APVMA 2000b
		0.53-1.95	3.8	4	77-242	148.5	4	0.53-1.95									EPA 1998l; EPA 1999d; EU 2005d; EU 2005e
		1.21-13.6	4.6	5	67.2-316.3	172.4	5	0.68-6.4	2.4	5	50.9-148.8	91.7	5	0.75-0.89	0.81	5	EU 2005d; EU 2005e; EFSA 2005n
615M01	cinidon-ethyl				869-5654		4	1.63-7.83		4							EU 2002d

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Transformation product	Parent pesticide	K_d			K_{oc}			K_f			K_{foc}			1/n			Reference(s)
		range	mean	n	range	mean	n	range	mean	n	range	mean	n	range	mean	n	
615M03[a]	cinidon-ethyl	0.11->18.1		4	0->2013		4										EU 2002d
CGA 193468[a]	clodinafop							4-5.4	4.6	3	238-365	285.3	3	0.73-0.89	0.8	3	EFSA 2005a
CGA 302371	clodinafop							0.62-1.1	0.87	3	25.1-81.6	49.7	3	0.84-0.96	0.9	3	EFSA 2005a
MNG	clothianidin										5.2-34.3	20.5	5	0.7-1.1		5	EU 2005f
TMG	clothianidin										525-3620	2459	5	0.73-0.85		5	EU 2005f
TNG	clothianidin										13.8-17.3	16	3	0.87-0.88		3	EU 2005f
TZMU	clothianidin										46.4-95.8	61.8	5	0.84-0.93		5	EU 2005f
TZNG	clothianidin										204.5-432.5	275.4	5	0.78-0.9		5	EU 2005f
chlorferon	coumaphos	91-191															PMRA 2003f
chloroacid cyanazine	cyanazine	0.08-0.23	0.17	4	7-11	9.7	4	0.21-0.42	0.3	4							Reddy et al. 1997
cyanazine amide	cyanazine	0.19-1.43	0.84	4	16-75	45.3	4	0.28-2.25	1.34	4							Reddy et al. 1997
desmethylpropanenitrile cyanazine	cyanazine	1.69-2.85	2	4	89-133	105.3	4	0.51-3.88	2.8	4							Reddy et al. 1997
deethylcyanazine	cyanazine	0.31-1.76	1.14	4	26-82	62.3	4	0.3-2.3	1.52	4							Reddy et al. 1997
hydroxyacid cyanazine	cyanazine	0.13-2.79	1.42	4	11-130	75.5	4	0.91-3.36	2.13	4							Reddy et al. 1997
CCIM	cyazofamid				327-1615			3.25-13.9			657-2900	753	4	0.81-1.13			EU 2002e; PMRA 2006a
CCIM-AM	cyazofamid				1560-2245			12.4-45.4			1941-3398	2396	4	0.92-1			EU 2002e; PMRA 2006a
CTCA	cyazofamid				308-1141			3.94-9.64			572-1357	836	4	0.84-1.15			EU 2002e; PMRA 2006a
2,4-dichloroaniline	cyclanilide				349-681	506.8	4										EU 2001b
						883[d]											EU 2001b
cyhalofop-acid	cyhalofop-butyl	1.41-1.95	1.68	2	176-195	185.5	2										EU 2002f
cyhalofop-amide	cyhalofop-butyl		0.4			50											EU 2002f
cyhalofop-diacid	cyhalofop-butyl	0.34-4.01	1.6	4	27-401	149.3	4										EU 2002f
CGA 249287[a]	cyprodinil							3.48-6.97		4	173-867	488	4	0.7-0.76	0.73	4	EFSA 2005b
CGA 275535	cyprodinil								8.3			1810			0.84		EFSA 2005b
decamethrinic acid	deltamethrin							0.27-0.59	0.41	3	10-44	26	3	0.84-0.96		3	EU 2002g
ethyl-m-hydroxyphenyl carbamate	desmedipham				124-335		4										EU 2004e
G27550	diazinon							0.13-0.18						0.86			EFSA 2006e
3,6-dichlorosalicylic acid	dicamba					504											Pearson et al. 1996
2,6-dichlorobenzoic acid	dichlobenil					<18[e]											Fava et al. 2005
4-chlorophenol	dichloroprop	1.15-2.61	1.82	4													Haberhauer et al. 2000

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Transformation product	Parent pesticide	K_d range	K_d mean	K_d n	K_{oc} range	K_{oc} mean	K_{oc} n	K_f range	K_f mean	K_f n	K_{foc} range	K_{foc} mean	K_{foc} n	1/n range	1/n mean	1/n n	Reference(s)
diclofop acid	diclofop-methyl	0.7-1.8	0.7	3	191-334	269.3	3										PSD 1991c
M23	dimethenamid & dimethenamid-P	0.05-0.35	0.15	6	3.5-17.2	7.7	6										EU 2003c; EFSA 2005c
M27	dimethenamid & dimethenamid-P	0.0-0.43	0.15	6	0.0-14.4	6.7	6										EU 2003c; EFSA 2005c
omethoate	dimethoate										16-87	41.3	3				EFSA 2006f
505M01	dimoxystrobin							0.02-1.21	0.24	7	2-35.5	13.1	7	0.74-0.93	0.87	7	EFSA 2005d
505M08	dimoxystrobin							0.09-0.69	0.35	6	7.8-133	38.8	6	0.91-0.99	0.95	6	EFSA 2005d
505M09	dimoxystrobin							0.14-1.77	0.65	7	9-119	46	7	0.81-0.92	0.86	7	EFSA 2005d
2,4-DNOP	dinocap	87-545	332	4				74.6-501	232	4	3930-50100	17421	4	0.85-1.13	1.01	4	EU 2007a
2,6-DNOP	dinocap	85-169	124	4				50-185	133	4	151-12900	8381	4	0.92-1.09	1.02	4	EU 2007a
DCPMU	diuron							3.5-15.6		4	498-1358		4	0.74-0.76		4	EFSA 2005e
DCPU	diuron							4.22-12.02		4	527-861		4	0.76-0.8		4	EFSA 2005e
m-CPDMU	diuron							2.3-8		3	139-418		3	0.69-0.78		3	EFSA 2005e
endosulfan sulphate	endosulfan					<12[a]											Fava et al. 2005
2-hydroxyethylphosphonic acid	ethephon										1464-5656	2733	4				EFSA 2006g
												12055[d]					EFSA 2006g
AE F136086	ethoxysulfuron				27-55												EU 2002h
metabolite R-3	etoxazole							47-183		3	3359-6295	5266	3	0.92-0.96		3	EU 2004f
metabolite R-4	etoxazole							3.02-10.4		3	216-360	294	3	0.9-0.93		3	EU 2004f
metabolite R-7	etoxazole							14-98		3	1125-7540	3665	3	0.87-0.93		3	EU 2004f
metabolite R-8	etoxazole							1.24-4.56		3	103-351	220	3	0.79-0.86		3	EU 2004f
metabolite R-11	etoxazole							0.32-1.34		3	23-46	32.6	3	0.65-0.92		3	EU 2004f
metabolite R-13	etoxazole							82-1082		3	13670-83230	44480	3	0.72-1		3	EU 2004f
IN-JS940	famoxadone				33-591	330	4	0.34-2.35		3	18-308	169	3	0.67-0.92		3	EU 2002i; PMRA 2003h
IN-KF015	famoxadone	1.37-14	6.5	4	130-1300	505	4										EU 2002i; PMRA 2003h
IN-KZ007	famoxadone				1238-34423	13705	4	17.5-21.6		3	1130-3942	2110	3	0.55-1.02		3	EU 2002i; PMRA 2003h
RPA412636	fenamidone							0.11-0.88	0.41	8	17-36	27	8	0.81-0.92	0.86	8	EU 2003d; PMRA 2007e
									0.64[d]			28[d]			0.96[d]		EU 2003d; PMRA 2007e
RPA412708	fenamidone							0.26-0.65	0.42	5	21-52	34.5	4	0.85-0.93	0.88	4	EU 2003d; PMRA 2007e
									0.51[d]			15[d]			0.97[d]		EU 2003d; PMRA 2007e

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Transformation product	Parent pesticide	K_d range	K_d mean	K_d n	K_{oc} range	K_{oc} mean	K_{oc} n	K_f range	K_f mean	K_f n	K_{foc} range	K_{foc} mean	K_{foc} n	1/n range	1/n mean	1/n n	Reference(s)
RPA413255	fenamidone							3.16-9.01	6.15	4	261-632	491.3	4	0.87-0.93	0.89	4	EU 2003d
									11.07[d]			326[d]			0.95[d]		EU 2003d
fenamiphos sulfone	fenamiphos							0.33-4.98		5	52.4-311						EFSA 2006h
		1.09-2.63															Oliver et al. 2005
fenamiphos sulfone phenol	fenamiphos							1.09-9.84		16	31-207						EFSA 2006h
fenamiphos sulfoxide	fenamiphos							0.71-3.6		3	44.8-225						EFSA 2006h
		0.4-1.78			49-125												Oliver et al. 2005
fenamiphos sulfoxide phenol	fenamiphos							0.15-7.88		16	12.5-166						EFSA 2006h
WAK 7004	fenhexamid	10.1-32.1		4	2327-5037		4										PMRA 2003b
3-methyl-4-nitrophenol	fenitrothion							2.42-7.84	5.95	3	270-303	285	3	0.71-0.81		3	EFSA 2006i
chlorobenzoxazolone	fenoxaprop-P							2.85-7.02	5.7	5				0.77-0.86	0.82	5	EFSA 2007d
MB 45950	fipronil							28.1-100	5.7	5	1695-5621	3911.4	5	0.93-1.05		5	PSD 2004a; EFSA 2006j
MB 46136	fipronil							26.6-148.4	66.3	5	1448-6745	4208.6	5	0.95-1.14	1.02	5	PSD 2004a; EFSA 2006j
MB 46513	fipronil										1150-1498	1290	5	0.92-0.94		5	EFSA 2006j
RPA 200766	fipronil							0.86-4.86	2.7	5	96-203	167.4	5	0.89-0.94	0.91	5	PSD 2004a; EFSA 2006j
5-hydroxy-XDE-570	florasulam	0.16-0.72															PMRA 2001c
		0.07-1.73	0.38	6							7-32	18	6	0.88-1.1		6	EU 2002j
ASTCA	florasulam	0.26-1.1	0.71	10	24-110	53.1	10										EU 2002j
DFP-ASTCA	florasulam	0.3-1.87	1.17	10	27-159	83	10										EU 2002j
compound V	fluazinam	4.3-26		6	450-1667		6										PMRA 2003j
compound XII	fluazinam	5-67		4	1284-3784		4										PMRA 2003j
2-trifluoromethoxy benzenesulfonamide	flucarbazone							0.13-1.59	0.86	2	50-50.2	50.1	2	0.9-0.92	0.91	2	Koskinen et al. 2006
CGA 192155	fludioxonil							0.06-0.28	0.21	4	11.7-42.4	23.5	4	0.77-0.84	0.8	4	EFSA 2007e
CGA 339833	fludioxonil							0.01-0.11	0.06	4	1.94-5.79	4.03	4	0.07-1.08	0.73	4	EFSA 2007e
CGA 265378	fludioxonil	36-111	68.3	4	0.65-0.83	0.75	4										EFSA 2007e
oxalate	flufenacet										7-23	14	4	0.82-1.42	1.04	4	EU 2003e
sulfonic acid	flufenacet										6-19	12.5	4	0.86-1.18	0.99	4	EU 2003e
M40	fluoxastrobin										37-87	59	4	0.86-0.95	0.9	4	EFSA 2005f
M48*	fluoxastrobin										14-181.5	60.3	4	0.92-0.98	0.95	4	EFSA 2005f
JV460	flupyrsulfuron-methyl				65-106	83.3	3				148-202	182	3				EU 2001c

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KC576	flupyrsulfuron-methyl				22-48	36.7	3				19-26	22	3				EU 2001c
KY374[a]	flupyrsulfuron-methyl				3-39	16.5	6										EU 2001c
fluroxypyr	fluroxpyr-meptyl	1.7															Tomlin 2000
TFAA	flurtamone	0.3-11			3.2-27.5	22.9											EU 2003f
TFMBA	flurtamone							0.36-1.94			15-52	32.5		0.52-0.81			EU 2003f
IN-F7321	flusilazole				164-822	532.3	4										EU 2007b
IN-H9933	flusilazole				8-22	16.5	4										EU 2007b
phthalimide[a]	folpet	1.92-12.98		3				2.49-15.6		3	72-385	208.7	3	0.84-0.89		3	EFSA 2006k
AE F092944	foramsulfuron & mesosulfuron							1.05-81.3	14.8	8	89-11289	1860.6	8	0.52-0.86	0.67	8	EU 2002k; PMRA 2003k
								2.47-16.5		5	89-917	447	5	0.62-0.86	0.72	5	EU 2004h
AE F130619	formasulfuron							0.36-2.98	1.5	4	40-144	72.8	4	0.9-0.94	0.93	4	EU 2002k; PMRA 2003k
AE F153745	formasulfuron				35-63	49.3	3										EU 2002k; PMRA 2003k
						48[d]											PMRA 2003k
3-formamidophenyl methylcarbamate	formetanate							0.69-3.15	1.65	4	68-142	107	4	0.86-0.92	0.9	4	EFSA 2006l
N'-(3-hydroxyphenyl)-N'N-dimethylformamidine	formetanate							1.79-40.2	15.3	4	368-1289	801	4	0.93-0.9	0.87	4	EFSA 2006l
3-hydroxyformanilide	formetanate							1.59-9.3	5.2	4	253-337	298	4	0.85-0.91	0.87	4	EFSA 2006l
3-aminophenyl-N-methylcarbamate	formetanate							0.76-2.3	1.3	3	40-70	57	3	0.66-0.88	0.78	3	EFSA 2006l
BESoP	fosthiazate	0.18-0.38		3													EU 2003g
metabolite M01	fuberidazole				13-15	14	3	2.26-4.53	3.7	3	257-308	278	3	0.77-0.79	0.78	3	EFSA 2007f
HOE 35956	glufosinate ammonium		0.4			16											PSD 1990f
MPA	glufosinate ammonium							0.16-1.1	0.54	6				0.71-0.97	0.86	6	EFSA 2005g
MPP	glufosinate ammonium							0.22-22	5.4	6				0.85-0.98	0.9	6	EFSA 2005g
aminomethylphosphonic acid	glyphosate glyphosate trimesium	15-1554	310	6							1160-24800	8026.7	6	0.75-0.9	0.8	6	EU 2002l
DE-535 phenol	haloxyfop-P	6.53-17.7		7	658-968		7										EFSA 2006m
DE-535 pyridinol	haloxyfop	0.33-0.8		7	23.4-67.8		7										EFSA 2006m
DE-535 pyridinone	haloxyfop	0.26-0.5		7	18.5-46.3		7										EFSA 2006m
CL 312,622	imazamox							0.64-1.81		6	27-279	123	6	0.9-0.97	0.94	6	EU 2002m

Table A3. The adsorption of pesticide transformation products in environmental systems (Chapter 2)

Transformation product	Parent pesticide	K_d range	K_d mean	K_d n	K_{oc} range	K_{oc} mean	K_{oc} n	K_f range	K_f mean	K_f n	K_{foc} range	K_{foc} mean	K_{foc} n	1/n range	1/n mean	1/n n	Reference(s)
CL 354,825	imazamox							1.97-18.2		6	331-1624	1224	6	0.68-0.89	0.79	6	EU 2002m
imidacloprid-guanidine	imidacloprid							29.8-156	83.9	3	2129-3805	3200.3	3	0.85-0.88	0.87	3	Cox et al. 1997
imidacloprid-guanidine-olefin	imidacloprid							32.4-116	68	3	2314-3083	2742	3	0.82-0.87	0.85	3	Cox et al. 1997
imidacloprid-urea	imidacloprid							2.93-8.67	5	3	189-211	203	3	0.82-0.85	0.84	3	Cox et al. 1997
IN-JT333	indoxacarb	96-241		4	8200-25000	17300	4										Strek et al. 2007
IN-JU873	indoxacarb							56-605		5	5417-31750	13167	5	0.94-1.12	1.02	5	Strek et al. 2007
IN-KG433	indoxacarb							1.2-8.7		5	275-395	314	5	0.88-0.95	0.92	5	Strek et al. 2007
IN-KT413	indoxacarb							1-10.3		4	204-469	344	4	0.83-1.01	0.95	4	Strek et al. 2007
IN-MK638	indoxacarb							0.9-2.6		5	67-300	151	5	0.76-0.94	0.95	5	Strek et al. 2007
IN-MK643	indoxacarb							1.3-4.2		5	189-353	269	5	0.77-0.83		5	Strek et al. 2007
AE F059411	iodosulfuron-methyl							0.3-1.57	0.66	4	15.4-172	70.8	4	0.84-0.91	0.86	4	EU 2003h; PMRA 2004f
AE F161778	iodosulfuron-methyl					~60											EU 2003h
metsulfuron-methyl	iodosulfuron-methyl							0.07-0.53	0.19	7	2.9-26.5	12.3	7	0.86-0.98	0.92	7	EU 2003h; PMRA 2004f
3,5-di-iodo-4-hydroxybenzamide	ioxynil & ioxynil octanoate							0.9-5.7	3.1	4	64-475	213.5	4	0.8-1.04	0.92	4	EU 2004g
3,5-di-iodo-4-hydroxybenzoic acid	ioxynil & ioxynil octanoate							0.48-9.44	3.9	4	72-786	266.3	4	0.52-0.9	0.68	4	EU 2004g
RP 30228	iprodione										6608-58120			1.2-2.6			EU 2002n
PMPA	iprovalicarb	0.67-11.09	4.2	4	118-575	290.3	4										EU 2002o
desmethylisoproturon	isoproturon							1.07-4.4		4	84-232	147	4				EU 2002p
RPA 202248	isoxaflutole				94-159	129.8	4										PMRA 2000e
						135[d]											PMRA 2000e
											54-159	108	8		0.941	8	EU 2003i
RPA 203328	isoxaflutole				47-100	80	4										PMRA 2000e
						23[d]											PMRA 2000e
kresoxim-methyl acid	kresoxim-methyl	0.55-0.62	0.59	2	17-69	37.4	4							0.91-0.94	0.93	2	PSD 1997c; EU 1998; PMRA 2003c
compound XV	*lambda*-cyhalothrin				36000-61000	44000	6										EU 2001d
ethylenethiourea	mancozeb, maneb, metiram & zineb	0.0006-0.051	0.035	2				0.51-1.14	0.76	4	34-146	69.7	4	0.33-0.55	0.44	4	EU 2005h; EU 2005i
		0.01-0.05			1-3												PSD 2004b
ethyleneurea	mancozeb & maneb	0.1-0.44		2	5.4-44.1		2										EU 2005i

Table A3. The adsorption of pesticide transformation products in environmental systems (Chapter 2)

Transformation product	Parent pesticide	K_d			K_{oc}			K_f			K_{foc}			1/n			Reference(s)
		range	mean	n	range	mean	n	range	mean	n	range	mean	n	range	mean	n	
2-methyl-4-chlorophenol	MCPA	1.05-3.72	2.29	4		93[a]											Haberhauer et al. 2000; Fava et al. 2005
MCPA[a]	MCPB				10-157	74	8										EU 2005k
AE F099095	mesosulfuron							2.33-42.8			141-1360	576	3	0.83-0.86	0.84	3	EU 2004h
AE F154851	mesosulfuron							0.75-3.1			46-98	68	3	0.92-0.95	0.94	3	EU 2004h
AMBA	mesotrione										22-158	77	4				EU 2003l
CGA62826	metalaxyl-M	3-72			1-11.4			0.02-0.9									EU 2002r
methiocarb methoxy sulfone	methiocarb	0.9-2.57	1.8	4							123.2-252	189	4	0.84-0.86	0.88	4	EFSA 2006n
methiocarb sulfone phenol	methiocarb	0.62-1.54	0.99	4							86.3-163	123	4	0.84-0.9	0.88	4	EFSA 2006n
methiocarb sulfoxide	methiocarb					31.3											EFSA 2006n
methiocarb sulfoxide phenol	methiocarb	0.19-0.66	0.48	4							26.7-101	50.7	4	0.89-0.91	0.9	4	EFSA 2006n
methomyl oxime	methomyl										6.6-20	11.4	5	0.68-0.95		5	EFSA 2006o
2-ethyl-6-methylaniline	metolachlor					197											Fava et al. 2000
metolachlor ethane sulfonic acid	metolachlor					195											Aga and Thurman 2001
CGA-51202	metolachlor & S-metolachlor	0.13-9.99		7	2.82-62	12.2	7	0.04-0.17	0.11	2							EPA 1995f; EU 2004k
CI 377160	metrafenone							62.1-264.1	105.8	5	2199-21649	6499	5	0.98-1.13	1.01	5	EFSA 2006p
deaminated diketo metribuzin	metribuzin							0.13-0.51	0.33	4	26.6-36.4	32.6	4	0.86-1.04	0.94	4	EPA 1998i; EFSA 2006q
diketo metribuzin	metribuzin							0.15-0.95	0.52	4	42.9-55.8	48.2	4	0.91-1	0.95	4	EPA 1998i
IN-A4098	metsulfuron-methyl, thifensulfuron-methyl & tribenuron-methyl	0.2-6.9		11	17-226	98	7	0.26-6.8		4							EU 2000c; EU 2001g; EFSA 2004
saccharin	metsulfuron-methyl & propoxycarbazone				5.7-10.6	8.9	4	0.03-0.27		4							EU 2000c
		0.02-0.25		5	4.6-15.5	5.2[c]	5										EU 2003p
hexamethyleneimine	molinate	1.64-7.23	4.9	5	226-603	426.2	5										EU 2003m
molinate sulfoxide	molinate	0.78-2.81	1.9	5	93-234	168.8	5										EU 2003m
ADMP	nicosulfuron							0.71-1.7	1.1	4	42-60	51.5	4	0.82-0.92	0.87	4	PSD 2000c; PMRA 2008
ASDM	nicosulfuron							0.05-0.24	0.12	4	2.3-7.7	5.7	4	0.81-1.07	0.91	4	PSD 2000c; PMRA 2008
AUSN	nicosulfuron							0.3-0.9	0.55	4	13-39	27.5	4	0.91-0.98	0.96	4	PSD 2000c; PMRA 2008
UCSN	nicosulfuron	0.02-0.09	0.06	4	1.1-5.6	2.7	4										PSD 2000c; PMRA 2008
desmethyl norflurazon	norflurazon							22.1-41.4									EPA 1996f
RP017272	oxadiargyl					856											EU 2002s

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Transformation product	Parent pesticide	K_d			K_{oc}			K_f			K_{foc}			1/n			Reference(s)
		range	mean	n	range	mean	n	range	mean	n	range	mean	n	range	mean	n	
RP025496	oxadiargyl					468											EU 2002s
IN-A2213	oxamyl	0.05-0.2	0.11	5	4-11	7	5	0.05-0.2	0.11	5	4-10	7	5	0.87-1.24	1.03	5	EFSA 2005h
IN-D2708	oxamyl	0.03-0.31	0.11	5	2-10	6	5	0.05-0.39	0.17	5	6-14	10	5	0.53-0.76	0.67	5	EFSA 2005h
IN-N0079	oxamyl	0.03-0.31	0.11	5	2-25	8	5										EFSA 2005h
C1801	oxasulfuron				54-213	146	3										EU 2002t
CGA 27913	oxasulfuron				3-6	4	3										EU 2002t
MET-42	pethoxamid		4.15		1.29-2.97	2.13	2	0.04-0.1	0.7	2							EU 2006a
MHPC	phenmedipham	0.57-4.8									212-470	220	4	0.52-0.85	0.74	4	EU 2004i
phorate sulfone	phorate				71-91												PMRA 2003a
phorate sulfoxide	phorate				172-210												PMRA 2003a
CL 153815	picolinafen	6.3-16.2		4	160-783	440	4										EU 2002u; PMRA 2003m
M2	pinoxaden	0.06-0.28	0.15	5	4.2-27	13.1	5										PMRA 2006b
M3	pinoxaden	0.12-0.86	0.5	5	23-48	31.6	5										PMRA 2006b
R31805*	pirimicarb										130-80000	14873	6	0.9-0.95	0.92	6	EFSA 2005i
R34836	pirimicarb										33.6-4320	927	6	0.83-0.93	0.9	6	EFSA 2005i
R34865	pirimicarb										179-9650	2940	6	0.62-0.85	0.76	6	EFSA 2005i
R34885	pirimicarb										57-867	269	6	0.9-0.95	0.92	6	EFSA 2005i
2,4-bis(isopropylamino)-6-hydroxy-s-triazine	prometryn							0.65-7.1									EPA 1996g
2-amino-4-isopropylamino-6-methylthio-s-triazine	prometryn							0.63-1.43									EPA 1996g
RH24580	pronamide	1.3-2.4			96-210												EPA 1994f
RH24644	pronamide	2.3-9.9			993-3910												EPA 1994f
propachlor oxanilic acid	propachlor	0.03-0.08	0.05	4	2-10	6.8	4										EPA 1998j
propachor sulfonic acid	propachlor	0.03-0.07	0.05	4	3-7	5.3	4										EPA 1998j
3,4-dichloroaniline	propanil					258											Fava et al. 2005
Ro 17-3102	propaquizafop							2.36-9.29	5.79	4	347-472	411.3	4	0.82-0.88	0.85	4	PSD 1994n
1,2,4-triazole	propiconazole, prothioconazole & tebuconazole				43-202		5										EU 2003n
					68-251												PMRA 2007g
					21.1-126.7												PMRA 2006e

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Transformation product	Parent pesticide	K_d			K_{oc}			K_f			K_{foc}			1/n			Reference(s)
		range	mean	n	range	mean	n	range	mean	n	range	mean	n	range	mean	n	
CGA 118 245	propiconazole				101-166		5										EU 2003n
propylene urea	propineb	0.17-0.63	0.44	4	13-26	18	4										EU 2003o
2,4-dihydro-5-propoxy-4-methyl-3H-1,2,4-triazol-3-one	propoxycarbazone							0.11-2.65	1.4	2	42.3-93.6	68	2	0.9-1.02	0.96	2	Koskinen et al. 2006
4-hydroxy saccharin	propoxycarbazone	7.5-46.3		5	456.9-2872.7	2033.8	5										EU 2003p
N-methyl propoxy triazolinone	propoxycarbazone	0.22-1.22		5	8.9-75.5	20.6	5										EU 2003p
N-methyl propoxy triazolinone amide	propoxycarbazone	0.26-3.9		5	10.4-551.5	99.9	5										EU 2003p
2-(3,5-dichlorophenyl)-4,4-dimethyl-5-methyleneoxazoline	propyzamide	2.3-56		6	993-3910	1894	6										EU 2003q
N-(1,1-dimethylacetonyl)-3,5-dichlorobenzamide	propyzamide	0.3-2.4		6	96-210	153	6										EU 2003q
prosulfocarb sulfoxide	prosulfocarb	1.23-2.55	1.9	3	61-88	70.7	3	1.02-1.98	1.5	3	50-68	56.7	3	0.9-0.91	0.91	3	EFSA 2007g
CGA 150829	prosulfuron & triasulfuron				55-281	144	4										EU 2000d; EU 2002v
CGA 159902	prosulfuron				48-96	77	4	0.4-1.24	0.75	4							EU 2002v
CGA 300406	prosulfuron				43-126	66.8	4	0.49-1.28	0.69	4							EU 2002v
CGA 325025	prosulfuron				60-238	123	4	1-1.02	1.01	4							EU 2002v
CGA 325030	prosulfuron				18-41	21	4										EU 2002v
CGA 32508	prosulfuron				11-31	20	5										EU 2002v
CGS 349707	prosulfuron				37-52	45	3										EU 2002v
prothioconazole-desthio	prothioconazole				419-549						523-625	575.4	4	0.79-0.83	0.81	4	PMRA 2007g; EFSA 2007h
prothioconazole-S-methyl	prothioconazole	15.6-64.1		4	2234-3779						1974-2995	2556	4	0.85-0.91	0.88	4	PMRA 2007g; EFSA 2007h
prothioconazole-thiazocine	prothioconazole					129											PMRA 2007g
CGA 180777	pymetrozine				5-49												PMRA 2002
CGA 249257	pymetrozine				9-30												PMRA 2002
CGA 359009	pymetrozine				284-436												PMRA 2002
GS23199	pymetrozine				31-48												PMRA 2002
BF 500-3	pyraclostobin				4240->5000												PMRA 2003n
BF 500-5	pyraclostobin				340-1163												PMRA 2003n
BF 500-6	pyraclostobin	79-610			3160-71300												EU 2004j
BF 500-7	pyraclostobin	98-738			3920-147600												EU 2004j

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Transformation product	Parent pesticide	K_d range	K_d mean	K_d n	K_{oc} range	K_{oc} mean	K_{oc} n	K_f range	K_f mean	K_f n	K_{foc} range	K_{foc} mean	K_{foc} n	1/n range	1/n mean	1/n n	Reference(s)
E-1	pyraflufen-ethyl				81-197		3	2.21-3.02		3							EU 2002w
E-2	pyraflufen-ethyl				1424-2179		3	26.2-52.7		3							EU 2002w
E-3	pyraflufen-ethyl				3098-4354		3	52.2-114.6		3							EU 2002w
AE B197555	pyrasulfotole							0.01-0.03			1-2			0.53-0.86			PMRA 2007b
6-chloro-3-phenyl-pyridazin-4-ol[a]	pyridate	0.5-3.5			20-188												PMRA 1991a; EU 2001e
2-amino-4,6-dimethylpyrimidine[a]	pyrimethanil							1.24-5.2	2.85	6	56-240	144	6	0.7-0.82	0.78	6	EFSA 2006r
BH518-5	quinmerac							0.51-1.49	1.06	4	28-211	88.8	4	0.88-1.28	1.07	4	PSD 1998c
BH518-2	quinmerac							0.43-2.38	1.42	4	53-98	73.5	4	0.77-0.83	0.8	4	PSD 1998c
IN-70941	rimsulfuron							0.27-1.85	0.74	4	34-116	60.8	4	0.92-0.96	0.94	4	EFSA 2005j
IN-70942	rimsulfuron							1.07-3.12	2.12	4	145-223	194.3	4	0.84-0.85	0.85	4	EFSA 2005j
IN-E9260	rimsulfuron							0.18-1.37	0.5	4	16-86	39.8	4	0.93-1.08	0.99	4	EFSA 2005j
CP 240659[a]	silthiofan	0.76-2.14		3	77-135		3	0.61-1.51		3							EU 2003r
hydroxysimazine	simazine	1.4-39			296-2360												PSD 1992e
CGA 354743	S-metolachlor	0.27-0.54		3	3-22	9[c]	7										EU 2004k
CGA 376944	S-metolachlor	0.24-0.55		3	8-12	10[c]	3										EU 2004k
CGA 40172	S-metolachlor	2.21-6.98		3	143-204	182[c]	3										EU 2004k
CGA 41507	S-metolachlor	2.88-5.56		3	81.3-93.8	84.9[c]	3										EU 2004k
2,4-dichlorobenzoic acid	spirodiclofen							0.05-0.12	0.07	4	4.7-8.8	7.2	4	0.05-0.82	0.26	4	EFSA 2007i
BAJ 2510	spirodiclofen				11.2-28.6												PMRA 2006c
BAJ 2740-dihydroxy	spirodiclofen							0.1-1.1	0.7	3	8.9-105	51.4	3	0.85-0.9	0.87	3	PMRA 2006c; EFSA 2007i
BAJ 2740-dioxoketone	spirodiclofen					3720											PMRA 2006c
BAJ 2740-enol	spirodiclofen							0.06-0.37	0.21	4	11.2-28.6	17.8	4	0.9-1.01	0.94	4	EFSA 2007i
BAJ 2740-ketohydroxy	spirodiclofen				612-2722												PMRA 2006c; EFSA 2007i
DCBA	spirodiclofen				4.7-21.8												PMRA 2006c
BSN 2060-4-carboxy	spiromesifen		0.07														PMRA 2007c
BSN 2060-enol (M01)	spiromesifen	0.02-0.05									1.2-8.3	4.2	4	0.72-0.93	0.82	4	PMRA 2007c; EFSA 2007j
M09	spiromesifen					3											EFSA 2007j
aminopyrimidine	sulfosulfuron	2.32-2.99			260-400												PMRA 1998; EU 2002x
		18.6-165.2	91.9	2	1042.4-8278	4660.2	2										PMRA 1998; EU 2002x

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sulfosulfuron desmethyl	sulfosulfuron	0.32-0.43			36.7-104.4												PMRA 1998; EU 2002x
		0.66-0.73			37.3-116												PMRA 1998; EU 2002x
sulphonamide	sulfosulfuron	0.52-2.07			60.9-260.5	163	4										PMRA 1998; EU 2002x
RH-112651	tebufenozide				76-156												PMRA 1996b
2,3,5,6-tetrachloroaniline	tecnazene				5102-26700	12662.3	4	20.4-1009.3	393.3	4							PSD 1995p
DP-1	tepraloxydim				48-1107	252.5	6	0.47-3.87									PMRA 2004b; EU 2004l
DP-2	tepraloxydim	0.34-13.7			22-3561												PMRA 2004b
					63-4193	791.3	6	0.35-14.7									EU 2004l
M02	thiacloprid										166-438	258	5	0.76-0.91		5	EU 2004m
M30	thiacloprid										11.9-26.2	19.8	5	0.91-0.98		5	EU 2004m
M34	thiacloprid				2.94-6.27	5.02	4										EU 2004m
CGA 322704	thiamethoxam				63-77	70	3										EU 2006b
					74-382												PMRA 2007d
CGA 353042	thiamethoxam				199-1451												PMRA 2007d
CGA 355190	thiamethoxam				37.6-187.5	91.5	6										EU 2006b; PMRA 2007d
NOA 404617	thiamethoxam				11-73												PMRA 2007d
NOA 407475	thiamethoxam				433-1550	761.2	6										EU 2006b; PMRA 2007d
IN-L9225	thifensulfuron-methyl				6.9-13.5	11.2	3										EU 2001g
IN-L9226	thifensulfuron-methyl				34-199	111	3										EU 2001g
IN-W8268	thifensulfuron-methyl				2.6-43												EU 2001g
methomyl	thiodicarb	0.2-1.4	0.8	4							13.3-42.8	25.2	5	0.82-0.89	0.86	5	EPA 1998k; EFSA 2005k
carbendazim	thiophanate-methyl	0.45-88.2				2100											EPA 2001c
DM-TM	tolclofos-methyl	0.18-0.33	0.27	3	11-22.2	15	3										EFSA 2005l
dimethylaminosulfotoluidide	tolyfluanid	0.41-1.73	0.98	4							56-118	76.4	4	0.89-0.93		4	EFSA 2005m
M670H05	topramezone										3-14						PMRA 2006d
M670H10	topramezone										291-5676						PMRA 2006d
triazamate metabolite II	triazamate	0.28-0.48	0.4	5	23-314	102	5										PSD 1998d
triazamate metabolite III	triazamate	0.45-0.7	0.59	5	34-493	150.4	5										PSD 1998d
triazamate metabolite IV	triazamate	0.34-0.53	0.45	5	28-376	115	5										PSD 1998d
IN-00581	tribenuron-methyl	0.2-0.5		3	12-20	15	3	0.2-0.3	0.3	3							EFSA 2004
IN-L5296	tribenuron-methyl	1.2-8		7	53-138	89	3	0.9-3.2	1.8	3							EFSA 2004

Table A3. The adsorption of pesticide transformation products in environmental systems (Chapter 2)

Transformation product	Parent pesticide	K_d			K_{oc}			K_f			K_{foc}			1/n			Reference(s)
		range	mean	n	range	mean	n	range	mean	n	range	mean	n	range	mean	n	
CGA-321113	trifloxystrobin							0.58-18.6		6	84-194	121	6	0.95-1.1	1	6	EU 2003s
					48-235												PMRA 2004h
CGA-357261	trifloxystrobin				389-567												PMRA 2004h
CGA-357276	trifloxystrobin				6587-9756												PMRA 2004h
CGA-373466	trifloxystrobin							0.17-3.07		5	30-166	88	5	1.01-1.26		5	EU 2003s; PMRA 2004h
NOA 413161	trifloxystrobin		0.042			4.2											EU 2003s
methyl saccharin	triflusulfuron-methyl							0.08-0.59	0.28	3	6.9-42	24.3	3	0.95-1.03	0.98	3	PSD 1995r
N,N-bis-demethyl triazine amine	triflusulfuron-methyl							0.37-3.42	1.14	5	32-213	97.6	5	0.93-1.05	0.97	5	PSD 1995r
N-demethyl triazine amine	triflusulfuron-methyl							0.59-4.88	1.9	5	51-300	199	5	0.8-0.9	0.86	5	PSD 1995r
triazine amine	triflusulfuron-methyl							1.05-10.1	3.8	5	89-2171	611	5	0.87-0.91	0.89	5	PSD 1995r
trinexapac acid	trinexapac-ethyl							1.54-16.4	5.7	4	145-609	415.8	4	0.85-0.92	0.89	4	PSD 1995s; EFSA 2005o
RPA 404766	triticonazole	1.3-2.49	2	4					3.63	4	35-133	82.8	4	0.83-0.88	0.85	4	EFSA 2005p
			2.15[d]						1.62[d]			62[d]			0.88[d]		EFSA 2005p
RPA 406341	triticonazole	0.82-3.31	1.9	4	61-163	122.5	4										PMRA 2004c
		1.71-4.78	3.09	4				0.82-2.65	1.9	4	61.163	123	3	0.84-0.87	0.86	4	EFSA 2005p
			4.27[d]						3.31[d]			127[d]			0.88[d]		PMRA 2004c EFSA 2005p
RPA 407922	triticonazole	3.88-19.1	12.3	4	467-1305	761	4										PMRA 2004c
		11.3-53.4	28.7	4				3.9-19.1	12.4	4	467-1305	761	4	0.71-0.83	0.78	4	EFSA 2005p
			14.9[d]						10.6[d]			407[d]			0.87[d]		PMRA 2004c EFSA 2005p
RH-127450	zoxamide							11.4-18.1	13.9	3	404-1156	669	3	0.45-0.6	0.52	3	EU 2004n
RH-163353	zoxamide							0.6-3.8	2.3	2	50-79	68	3	0.83-0.84	0.84	3	EU 2004n
RH-24549[e]	zoxamide							1.8-4.9	3.1	3	90.5-307.4	183	3	0.79-0.83	0.81	3	EU 2004n
RH-7281	zoxamide							3.4-25.3	13.3	5	815-1431	1224	5	0.9-1.07	0.97	5	EU 2004n

[a] – determined by HPLC

[b] – determined by column leaching

[c] – median value

[d] – sediment

[e] – pH dependent adsorption identified

Table A4. The occurrence of pesticide transformation products in environmental systems (Chapter 2)

Environmental compartment	Transformation product	Parent pesticide [a]	Concentration	Limit of detection	Country	Reference
Soil						
topsoil (0-30 cm)	3-chloralfyl alcohol	1,3-dichloropropene	ND	10 µg kg^{-1}	USA	Obreza and Ontermaa 1991
	2-chloro-2',6'-diethylacetanilide	alachlor	ND	10 µg g^{-1}	Germany	Heyer and Stan 1995
	2,6-diethylaniline	alachlor	ND	10 µg g^{-1}	Germany	Heyer and Stan 1995
	alachlor ethane sulfonic acid	alachlor	43.5 - 210 µg kg^{-1}	-	USA	Aga and Thurman 2001
			≤0.027 ppm	-	USA	EPA 1998b
			0.003 - 0.01 ppm	-	USA	EPA 1998b
	alachlor oxanilic acid	alachlor	≤0.047 ppm	-	USA	EPA 1998b
			0.005 - 0.058 ppm	-	USA	EPA 1998b
	alachlor sulfinylacetic acid	alachlor	≤0.039 ppm	-	USA	EPA 1998b
			0.002 - 0.017 ppm	-	USA	EPA 1998b
	alachlor DM-oxanilic acid	alachlor	≤0.061 ppm	-	USA	EPA 1998b
			0.006 - 0.048 ppm	-	USA	EPA 1998b
	cyanamide	amitrole	0.02 mg kg^{-1}	-	USA	EPA 1998b
	deethylatrazine	atrazine	< 12 - 60 µg kg^{-1}	-	USA	Mills and Thurman 1994
			14 ± 2 ppb	1 - 5 ppb	Canada	Khan and Saidak 1981
			< 1 - 15.3 µg kg^{-1}	-	Canada	Raju et al. 1993
			0.04 - 0.11 ± 0.01 µg g^{-1}	-	USA	Winkelmann and Klaine 1991
	deisopropylatrazine	atrazine	< 4 - 27 µg kg^{-1}	-	USA	Mills and Thurman 1994
			< 1 - 10.08 µg kg^{-1}	-	Canada	Raju et al. 1993
			0.01 - 0.02 µg g^{-1}	-	USA	Winkelmann and Klaine 1991
	hydroxyatrazine	atrazine	296 ± 27 - 378 ± 30 ppb	1 - 5 ppb	Canada	Khan and Saidak 1981
			< 1 - 52.1 µg kg^{-1}	-	Canada	Raju et al. 1993
			0.41 ± 0.08 - 0.5 µg g^{-1}	-	USA	Winkelmann and Klaine 1991
	deethylhydroxyatrazine	atrazine	47 ± 4 - 17 ± 2 ppb	1 - 5 ppb	Canada	Khan and Saidak 1981
	deisopropylhydroxyatrazine	atrazine	23 ± 2 - 64 ± 8 ppb	1 - 5 ppb	Canada	Khan and Saidak 1981
	reference compound 2	azoxystrobin	<0.05 µg kg^{-1}	-	Canada	PMRA 2000a
	reference compound 28	azoxystrobin	<0.05 µg kg^{-1}	-	Canada	PMRA 2000a
	reference compound 30	azoxystrobin	<0.05 µg kg^{-1}	-	Canada	PMRA 2000a
	benalaxyl M1	benalaxyl	0.3 - 0.7 mg kg^{-1}	-	-	EU 2004c
	benalaxyl M2	benalaxyl	< 0.1 mg kg^{-1}	-	-	EU 2004c

Table A4. The occurrence of pesticide transformation products in environmental systems (Chapter 2)

Environmental compartment	Transformation product	Parent pesticide [a]	Concentration	Limit of detection	Country	Reference
topsoil (0-30 cm) continued..	carbofuran	benfuracarb	< 1 - 6.3 mg kg^{-1}	-	Japan	PSD 1998a
	2-amino-N-isopropyl benzamide	bentazone	<0.1 ppm	-	Germany	EPA 2001a
			<0.05 ppm	-	USA	EPA 2001a
	SDS1449	chlorthal-dimethyl	ND - 0.11 kg ha^{-1}	0.01 ppm	USA	Niemczyk and Krause 1994
	SDS954	chlorthal-dimethyl	ND - 2.09 kg ha^{-1}	0.01 ppm	USA	Niemczyk and Krause 1994
	1-(2,4-dichlorophenyl) ethan-1-ol	chlorfenvinphos	ND	2 mg kg^{-1}	-	PSD 1994d
			0.3 mg kg^{-1} [c]	-	Belgium	PSD 1994d
			0.3 mg kg^{-1} [c]	-	Belgium	PSD 1994d
	2-hydroxy-4-chlorobenzoic acid	chlorfenvinphos	5.6±0.2 mg kg^{-1}	0.02 mg kg^{-1}	Belgium	PSD 1994d
			3.2 mg kg^{-1} [c]	-	Belgium	PSD 1994d
			4.7 mg kg^{-1} [c]	-	Belgium	PSD 1994d
			5.7 mg kg^{-1} [c]	-	Belgium	PSD 1994d
			5.0 mg kg^{-1} [c]	-	Belgium	PSD 1994d
	2,4-dichloroacetophenone	chlorfenvinphos	0.4 mg kg^{-1} [c]	-	Belgium	PSD 1994d
			0.4 mg kg^{-1} [c]	-	Belgium	PSD 1994d
			0.3 mg kg^{-1} [c]	-	Belgium	PSD 1994d
	2,4-dichlorophenacyl chloride	chlorfenvinphos	0.1 mg kg^{-1}	-	-	PSD 1994d
			3.5±0.2 mg kg^{-1}	0.02 mg kg^{-1}	Belgium	PSD 1994d
			4.8 mg kg^{-1} [c]	-	Belgium	PSD 1994d
			4.3 mg kg^{-1} [c]	-	Belgium	PSD 1994d
			3.5 mg kg^{-1} [c]	-	Belgium	PSD 1994d
			3.3 mg kg^{-1} [c]	-	Belgium	PSD 1994d
	2,4-dichlorobenzoic acid	chlorfenvinphos	7.3±0.3 mg kg^{-1}	0.02 mg kg^{-1}	Belgium	PSD 1994d
			4.7 mg kg^{-1} [c]	-	Belgium	PSD 1994d
			4.9 mg kg^{-1} [c]	-	Belgium	PSD 1994d
			7.4 mg kg^{-1} [c]	-	Belgium	PSD 1994d
			7.9 mg kg^{-1} [c]	-	Belgium	PSD 1994d
	2,4-dihydroxybenzoic acid	chlorfenvinphos	1.5±0.1 mg kg^{-1}	0.02 mg kg^{-1}	Belgium	PSD 1994d
			1.1 mg kg^{-1} [c]	-	Belgium	PSD 1994d
			1.3 mg kg^{-1} [c]	-	Belgium	PSD 1994d
	2,4-dihydroxybenzoic acid	chlorfenvinphos	2.5 mg kg^{-1} [c]	-	Belgium	PSD 1994d
			2.0 mg kg^{-1} [c]	-	Belgium	PSD 1994d
	dichlorobenzyl alcohol	chlorfenvinphos	0.5 mg kg^{-1} [c]	-	Belgium	PSD 1994d
	trichloroacetophenone	chlorfenvinphos	0.1 mg kg^{-1}	-	-	PSD 1994d
	3,5,6-trichloro-2-pyridinol	chlorpyrifos	0.09 - 1.01 mg kg^{-1} [b]	-	USA	APVMA 2000b
	3,5,6-trichloro-2-methoxypyridine	chlorpyrifos	0.01 - 0.06 mg kg^{-1} [b]			APVMA 2000b

Table A4. The occurrence of pesticide transformation products in environmental systems (Chapter 2)

Environmental compartment	Transformation product	Parent pesticide [a]	Concentration	Limit of detection	Country	Reference
topsoil (0-30 cm) continued..	cyanazine amide	cyanazine	<0.01 - 1.1 ppm	-	France and UK	Beynon et al. 1972a
			0.41 - 0.9 ppm	-	UK	Beynon et al. 1972b
	2-chloro-4-(1-carbonyl-1-methylethylamino)-6-amino-1,3,5-triazine	cyanazine	< 0.01 - 0.08 ppm	-	France and UK	Beynon et al. 1972a
	cyanazine acid	cyanazine	0.72 - 1.66 ppm	-	UK	Beynon et al. 1972b
	cyanazine hydroxy acid	cyanazine	0.1 - 0.79 ppm	-	UK	Beynon et al. 1972b
	2-[(4-amino-6-chloro(1,3,5-triazin-2-yl))amino]-2-methylpropanenitrile	cyanazine	< 0.01 - 0.02 ppm	-	UK	Beynon et al. 1972b
	(4-amino-6-chloro(1,3,5-triazin-2-yl))ethylamine	cyanazine	0.03 - 0.08 ppm	-	UK	Beynon et al. 1972b
	CCA	cypermethrin	1-10 ng g^{-1}	ng g^{-1} range	Germany	Class 1992
	3-phenoxybenzoic acid	cypermethrin	1-10 ng g^{-1}	ng g^{-1} range	Germany	Class 1992
	3-phenoxybenzaldehyde	cypermethrin	1-10 ng g^{-1}	ng g^{-1} range	Germany	Class 1992
	CGA 249287	cyprodinil	0.12 mg kg^{-1}	0.02 mg kg^{-1}	UK	PSD 1997a
			0.11 mg kg^{-1}	0.02 mg kg^{-1}	UK	PSD 1997a
			0.08 mg kg^{-1}	0.02 mg kg^{-1}	UK	PSD 1997a
			0.02 - 0.03 mg kg^{-1}	0.01 mg kg^{-1}	Switzerland	PSD 1997a
			0.05 mg kg^{-1} [b]	0.01 mg kg^{-1}	Switzerland	PSD 1997a
	melamine	cyromazine	0.05 - 1.4 mg kg^{-1}	-	Switzerland	PSD 1993c
	decamethrinic acid	deltamethrin	ND	0.01 mg kg^{-1}	USA	EU 2002g
	ethyl-m-hydroxyphenyl carbamate	desmedipham	ND - 0.59 mg kg^{-1}	0.005 mg kg^{-1}	USA	PSD 1993d
	o,p'-DDE	DDT	> 0.01 ± 0.01 µg g^{-1}	-	Australia	Van Zweiten et al. 2001
	p,p'-DDE	DDT	17.3 ± 1.6 µg g^{-1}	-	Australia	Van Zweiten et al. 2001
	o,p'-DDD	DDT	20.9 ± 4.9 µg g^{-1}	-	Australia	Van Zweiten et al. 2001
	p,p'-DDD	DDT	9.0 ± 1.0 µg g^{-1}	-	Australia	Van Zweiten et al. 2001
	diazoxon	diazinon	ND	0.001 ppm	UK	PSD 1991b
	3,6-dichlorosalicylic acid	dicamba	0.05 - 1.25 µg g^{-1}	0.005 µg g^{-1}	USA	Krueger et al. 1991
	2,5-dihydroxy-3,6-dichlorosalicylic acid	dicamba	0.03 - 0.1 µg g^{-1}	0.005 µg g^{-1}	USA	Krueger et al. 1991
	diclofop acid	diclofop-methyl	0.01- 0.28 mg kg^{-1}	-	USA	PSD 1991c
	p-chlorophenyl	diflubenzuron	<0.002 - 0.06 ppm	-	USA	EPA 1997a
	2,6-difluorobenzoic acid	diflubenzuron	ND - 0.01 ppm	-	USA	EPA 1997a
	DM2	diflufenican	ND - 20 ± 1 µg kg^{-1}	2 µg kg^{-1}	Belgium	Rouchaud et al. 1991
	DM3	diflufenican	ND - 26 ± 1 µg kg^{-1}	2 µg kg^{-1}	Belgium	Rouchaud et al. 1991
	DM4	diflufenican	ND - 23 ± 1 µg kg^{-1}	2 µg kg^{-1}	Belgium	Rouchaud et al. 1991
	2,4-difluoroaniline	diflufenican	ND	5 µg kg^{-1}	Belgium	Rouchaud et al. 1991

Table A4. The occurrence of pesticide transformation products in environmental systems (Chapter 2)

Environmental compartment	Transformation product	Parent pesticide [a]	Concentration	Limit of detection	Country	Reference
topsoil (0-30 cm) continued..	3-(trifluoromethyl)phenol	diflufenican	ND	5 µg kg^{-1}	Belgium	Rouchaud et al. 1991
	N-demethyldimefuron	dimefuron	0.1 mg kg^{-1} [b]	-	UK	PSD 1993e
	dimethoxon	dimethoate	0.01 - 0.561 ppm	-	USA	EPA 1999e
	$CONH_2$-fen	esfenvalerate	ND	0.01 mg kg_{-1}	UK and USA	EU 2000b
	RH-6467	fenbuconazole	5 µg kg^{-1} [b]	0.01 mg kg^{-1}	Germany	PSD 1995c
			0.016 mg kg^{-1}	0.01 mg kg^{-1}	USA	PSD 1995c
			0.047 mg kg^{-1} [b]	0.01 mg kg^{-1}	USA	PSD 1995c
	RH-9129	fenbuconazole	ND	0.01 mg kg^{-1}	Germany	PSD 1995c
			0.031 mg kg^{-1}	0.01 mg kg^{-1}	USA	PSD 1995c
			0.05 mg kg^{-1} [b]	0.01 mg kg^{-1}	USA	PSD 1995c
	RH-9130	fenbuconazole	ND	0.01 mg kg^{-1}	Germany	PSD 1995c
			0.01 mg kg^{-1}	0.01 mg kg^{-1}	USA	PSD 1995c
			0.063 mg kg^{-1} [b]	0.01 mg kg^{-1}	USA	PSD 1995c
	FBC 96912	fluquinconazole	0.13 mg kg^{-1} [b]	0.02 mg kg^{-1}	UK	PSD 1999b
			0.16 mg kg^{-1} [b]	0.02 mg kg^{-1}	UK	PSD 1999b
			0.18 mg kg^{-1} [b]	0.02 mg kg^{-1}	France	PSD 1999b
			0.19 mg kg^{-1} [b]	0.02 mg kg^{-1}	Germany	PSD 1999b
	fomesafen amine	fomesafen	<0.02 mg kg^{-1}	0.01 mg kg^{-1}	USA	PSD 1995f
	carbamoylphosphonic acid	foseamine-ammonium	1.3 - 8.6 ppm	-	-	EPA 1995d
	3-methyl phosphinico-proprionic acid	glufosinate ammonium	0.03 - 0.2 mg kg^{-1}	-		PSD 1990f
			ND - 0.03 mg kg^{-1}	< 0.05 mg kg^{-1}	-	PSD 1990f
	aminomethylphosphonic acid	glyphosate	0.6 ppm	-	USA	EPA 1993b
	2-hydroxyquinoxaline	quinalphos	ND - 64 ± 2 µg kg^{-1}	< 1 mg g^{-1}	India	Menon and Gopal 2003
	quinoxaline-2-thiol	quinalphos	ND - 35 ± 7 µg kg^{-1}	< 1 mg g^{-1}	India	Menon and Gopal 2003
	RP 30228	iprodione	0.47 ppm	-	USA	EPA 1998g
			0.01 - 0.08 ppm	-	USA	EPA 1998g
	RP 32490	iprodione	≤0.09 ppm	-	USA	EPA 1998g
	3-(3,4-dichlorophenyl)-1-methylurea	linuron	0.1 ppm	-	Canada	PSD 1995h
	3,4-dichloroaniline	linuron	1.4 ppm	0.1 ppm	-	PSD 1995h
			0.4 ppb	0.1 ppb	-	PSD 1995h
	3,3',4,4'-tetrachloroazobenzene	linuron	ND	0.1 ppm	-	PSD 1995h
			ND	0.1 ppb	-	PSD 1995h
	4-chloro-2-methylphenol	MCPA	5 - 6 mg kg^{-1} [b]	15 - 45 µg kg^{-1}	Spain	Crespin et al. 2001
	HOE 094270	mefenpyr-diethyl	0.0948 mg kg^{-1} [b]	0.007 mg kg^{-1}	Germany	PSD 1999a
	methiocarb sulfoxide	methiocarb	100 µg kg^{-1} [b]	10 µg kg^{-1}	Germany	PSD 1998b
	methiocarb sulfone	methiocarb	22 µg kg^{-1} [b]	10 µg kg^{-1}	Germany	PSD 1998b
	metolachlor ethane sulfonic acid	metolachlor	11.91 - 128 µg kg^{-1}	-	USA	Aga and Thurman 2001
	ATSA	metosulam	0.001 - 0.005 mg kg^{-1}	-	USA	PSD 1996c
	5-hydroxymetosulam	metosulam	0.001 - 0.005 mg kg^{-1}	-	USA	PSD 1996c

Table A4. The occurrence of pesticide transformation products in environmental systems (Chapter 2)

Environmental compartment	Transformation product	Parent pesticide [a]	Concentration	Limit of detection	Country	Reference
topsoil (0-30 cm) continued..	7-hydroxymetosulam	metosulam	0.001 - 0.005 mg kg^{-1}	-	USA	PSD 1996c
	2,4-bis(isopropylamino)-6-hydroxy-s-triazine	prometryn	0.322 - 0.735 ppm	-	USA	EPA 1996g
	2-amino-4-isopropylamino-6-methylthio-s-triazine	prometryn	0.025 - 0.066 ppm	-	USA	EPA 1996g
	propachlor oxanilic acid	propachlor	0.668 ppm [b]	-	USA	EPA 1998j
	propachlor sulfinylacetic acid	propachlor	0.201 ppm [b]	-	USA	EPA 1998j
	propachlor ethane sulfonic acid	propachlor	0.416 ppm [b]	-	USA	EPA 1998j
	hydroxypropachlor	propachlor	0.351 ppm [b]	-	USA	EPA 1998j
	norchloropropachlor	propachlor	0.101 - 0.14 ppm	-	USA	EPA 1998j
	propachlor methylsulfone	propachlor	0.046 ppm	-	USA	EPA 1998j
	6-chloro-3-phenyl-pyridazin-4-ol	pyridate	0.07 - 0.75 mg kg^{-1}	-	-	EU 2001e
	BH518-2	quinmerac	ND - 0.078 mg kg^{-1}	0.01 mg kg^{-1}	Germany	PSD 1998c
	BH518-5	quinmerac	ND - 0.078 mg kg^{-1}	0.01 mg kg^{-1}	Germany	PSD 1998c
	PP890	tefluthrin	0.02 - 0.1 mg kg^{-1}	0.01 mg kg^{-1}	USA	PSD 1991h
	2,3,5,6-tetrafluoro-4-methyl benzoic acid	tefluthrin	0.02 - 0.1 mg kg^{-1}	0.01 mg kg^{-1}	USA	PSD 1991h
	thiobencarb sulfoxide	thiobencarb	≤2 ppm	0.01 ppm	USA	EPA 1997e
	DMST	tolyfluanid	3.15 mg kg^{-1} [b]	0.1 mg kg^{-1}	Germany	PSD 1995q
	SAS 9256	triazoxide	0.64 mg kg^{-1}	0.04 mg kg^{-1}	Germany	PSD 1993n
	3,5,6-trichloro-2-pyridinol	triclopyr	0.131 ppm	63 weeks	-	EPA 1998l
	3,5,6-trichloro-2-pyridinol	triclopyr butoxyethyl ester	0.04 - 1.4 ppm	-	USA	EPA 1998l
	3,5,6-trichloro-2-methoxypyridine	triclopyr butoxyethyl ester	0.15 - 0.35 ppm	-	USA	EPA 1998l
	methyl saccharin	triflusulfuron-methyl	0.015 mg kg^{-1}	0.002 mg kg^{-1}	USA	PSD 1995r
	triazine amine B	triflusulfuron-methyl	0.041 mg kg^{-1}	0.002 mg kg^{-1}	USA	PSD 1995r
	N-demethyl triazine amine B	triflusulfuron-methyl	0.014 mg kg^{-1}	0.002 mg kg^{-1}	USA	PSD 1995r
	N,N-bis-demethyl triazine amine B	triflusulfuron-methyl	0.006 mg kg^{-1}	0.002 mg kg^{-1}	USA	PSD 1995r
	trinexapac acid	trinexapac ethyl	0.03 mg kg^{-1}	0.02 mg kg^{-1}	Switzerland	PSD 1995s
			0.06 mg kg^{-1}	0.02 mg kg^{-1}	Switzerland	PSD 1995s
			0.14 mg kg^{-1}	0.02 mg kg^{-1}	France	PSD 1995s
			0.13 mg kg^{-1} [b]	0.01 mg kg^{-1}	USA	PSD 1995s
			0.42 mg kg^{-1} [b]	0.01 mg kg^{-1}	USA	PSD 1995s
			0.7 mg kg^{-1} [b]	0.01 mg kg^{-1}	USA	PSD 1995s
			0.36 mg kg^{-1} [b]	0.01 mg kg^{-1}	USA	PSD 1995s
			0.302 mg kg^{-1} [b]	0.01 mg kg^{-1}	USA	PSD 1995s
subsoil (30 - 60cm)						
	3-chlorallyl alcohol	1,3-dichloropropene	ND	10 µg kg^{-1}	USA	Obreza and Ontermaa 1991
	alachlor ethane sulfonic acid	alachlor	80 - 142 µg kg^{-1}	-	USA	Aga and Thurman 2001
	dimethoxon	dimethoate	0.012 ppm	-	USA	EPA 1999e

Table A4. The occurrence of pesticide transformation products in environmental systems (Chapter 2)

Environmental compartment	Transformation product	Parent pesticide [a]	Concentration	Limit of detection	Country	Reference
subsoil (30 - 60cm) continued...	metolachlor ethane sulfonic acid	metolachlor	3.6 - 13.3 µg kg^{-1}	-	USA	Aga and Thurman 2001
	propachlor ethane sulfonic acid	propachlor	0.015 ppm [b]	-	USA	EPA 1998j
	BH518-2	quinmerac	ND - 0.01 mg kg^{-1}	0.01 mg kg^{-1}	Germany	PSD 1998c
	BH518-5	quinmerac	ND - 0.01 mg kg^{-1}	0.01 mg kg^{-1}	Germany	PSD 1998c
	N,N-bis-demethyl triazine amine B	triflusulfuron-methyl	0.004 mg kg^{-1}	0.002 mg kg^{-1}	USA	PSD 1995r
subsoil (60 - 90cm)						
	alachlor ethane sulfonic acid	alachlor	13.3 - 140 µg kg^{-1}	-	USA	Aga and Thurman 2001
			≤0.011 ppm	-	USA	EPA 1998b
	alachlor oxanilic acid	alachlor	≤0.023 ppm	-	USA	EPA 1998b
	metolachlor ethane sulfonic acid	metolachlor	18.7 - 122 µg kg^{-1}	-	USA	Aga and Thurman 2001
	CGA-40172	metolachlor	0.07 ppm	-	USA	EPA 1995f
	CGA-40919	metolachlor	0.21 ppm	-	USA	EPA 1995f
	CGA-50720	metolachlor	ND	-	-	EPA 1995f
	CGA-51202	metolachlor	0.11 ppm	-	-	EPA 1995f
	propachlor sulfinylacetic acid	propachlor	0.012 ppm [b]	-	USA	EPA 1998j
	propachlor oxanilic acid	propachlor	0.013 ppm [b]	-	USA	EPA 1998j
	BH518-5	quinmerac	ND - 0.01 mg kg^{-1}	0.01 mg kg^{-1}	Germany	PSD 1998c
	methomyl	thiodicarb	4 ppb [b]	-	USA	EPA 1998k
Vadose zone water						
	alachlor ethane sulfonic acid	alachlor	3 - 73 µg L^{-1}	0.5 µg L^{-1}	USA	Aga and Thurman 2001
	deethylatrazine	atrazine	0.3 µg L^{-1} [c]	0.04 µg L^{-1}	USA	Steinheimer and Scoggin 2001
			9 - 19 µg L^{-1} [b]	0.1 µg L^{-1}	USA	Fermanich et al. 1996
			0.76 - 1.48 µg L^{-1} [b]	0.04 µg L^{-1}	USA	Pashin et al. 2000
			15 - 29 µg L^{-1} [b]	-	USA	Mills and Thurman 1994
			4.7 - 22.1 µg L^{-1} [b]	0.02 µg L^{-1}	USA	Adams and Thurman 1991
	deisopropylatrazine	atrazine	0.6 µg L^{-1} [c]	0.04 µg L^{-1}	USA	Steinheimer and Scoggin 2001
			< 0.5 µg L^{-1}	0.2 µg L^{-1}	USA	Fermanich et al. 1996
			0.11 - 0.78 µg L^{-1}	0.03 µg L^{-1}	USA	Pashin et al. 2000
			7 - 15 µg L^{-1} [b]	-	USA	Mills and Thurman 1994

Table A4. The occurrence of pesticide transformation products in environmental systems (Chapter 2)

Environmental compartment	Transformation product	Parent pesticide [a]	Concentration	Limit of detection	Country	Reference
Vadose zone water continued...			< 0.02 µg L^{-1}	0.02 µg L^{-1}	USA	Adams and Thurman 1991
	didealkylatrazine	atrazine	0.2 - 1.25 µg L^{-1}	0.03 µg L^{-1}	USA	Pashin et al. 2000
	hydroxyatrazine	atrazine	0.08 - 0.37 µg L^{-1}	0.04 µg L^{-1}	USA	Pashin et al. 2000
	BH518-2	quinmerac	0.7 µg L^{-1} [b]	0.05 µg L^{-1}	Germany	PSD 1998c
	BH518-5	quinmerac	0.16 µg L^{-1} [b]	0.05 µg L^{-1}	Germany	PSD 1998c
Leachate column studies						
	2,6-diethylaniline	alachlor	1 µg L^{-1}	-	Italy	Fava et al. 2000
	2-chloro-2',6'-diethylacetanilide	alachlor	2.2 - 2.7 µg L^{-1}	-	Italy	Fava et al. 2000
	2-hydroxy-2',6'-diethylacetanilide	alachlor	0.8 µg L^{-1}	-	Italy	Fava et al. 2000
	2-ethyl-6-methylaniline	metolachlor	0.6 µg L^{-1}	-	Italy	Fava et al. 2000
	RH-6467	fenbuconazole	trace	-	-	PSD 1995c
	RH-9129	fenbuconazole	trace	-	-	PSD 1995c
	RH-9130	fenbuconazole	trace	-	-	PSD 1995c
lysimeter studies						
	aldicarb sulfone	aldicarb	1.5 µg L^{-1}	-	-	APVMA 2001
	aldicarb sulfoxide	aldicarb	0.23 µg L^{-1}	-	-	APVMA 2001
	benalaxyl M1	benalaxyl	4.68 - 4.87 µg L^{-1} [c]	-	Switzerland	EU 2004c
	benalaxyl M2	benalaxyl	4.53 - 7.83 µg L^{-1} [c]	-	Switzerland	EU 2004c
	2,6-dichlorbenzamide	diclobenil	14.2 - 80.4 ppb	-	Germany	EPA 1998e
	trifluoroethanoic acid	flurtamone	2.53 - 11.46 µg L^{-1}	-	UK	PSD 2000a
	RE 54488	flurtamone	0.03 - 0.05 µg L^{-1}	-	UK	PSD 2000a
	kresoxim-methyl acid	kresoxim-methyl	ND - 0.04 µg L^{-1}	0.01µg L^{-1}	Germany	PSD 1997c
			0.25 - 0.33 µg kg^{-1} (soil)		Germany	PSD 1997c
Surface water runoff						
	acetochlor oxanilic acid	acetochlor	ND - 0.08 µg L^{-1}	0.01 µg L^{-1}	USA	Ferrer et al. 1997
	alachlor ethane sulfonic acid	alachlor	ND - 48.84 µg L^{-1}	0.5 µg L^{-1}	USA	Aga and Thurman 2001
	alachlor oxanilic acid	alachlor	ND - 0.17 µg L^{-1}	0.01 µg L^{-1}	USA	Ferrer et al. 1997
	deethylatrazine	atrazine	0 - 10.33 µg L^{-1} [d]	-	France	Patty et al. 1997
			8 - 29 µg L^{-1} [b]	0.05 µg L^{-1}	USA	Thurman et al. 1994
			0.97 µg L^{-1} [c]	0.02 µg L^{-1}	USA	Blanchard and Donald 1997
	deisopropylatrazine	atrazine	0 - 12.14 µg L^{-1} [d]	-	France	Patty et al. 1997
	metolachlor ethane sulfonic acid	metolachlor	ND - 1.26 µg L^{-1}	0.5 µg L^{-1}	USA	Aga and Thurman 2001
			0.05 - 0.47 µg L^{-1}	0.01 µg L^{-1}	USA	Ferrer et al. 1997

Table A4. The occurrence of pesticide transformation products in environmental systems (Chapter 2)

Environmental compartment	Transformation product	Parent pesticide [a]	Concentration	Limit of detection	Country	Reference
	metolachlor oxanilic acid	metolachlor	ND - 0.29 µg L^{-1}	0.01 µg L^{-1}	USA	Ferrer et al. 1997
tile drain						
	deethylatrazine	atrazine	0.36 - 7.71 µg L^{-1}	0.01 µg L^{-1}	Canada	Muir and Baker 1976
	deisopropylatrazine	atrazine	0.01 - 0.78 µg L^{-1}	0.01 µg L^{-1}	Canada	Muir and Baker 1976
	cyanazine amide	cyanazine	< 0.04 - 3.3 µg L^{-1}	0.01 µg L^{-1}	Canada	Muir and Baker 1976
	deisopropylatrazine	cyanazine	0.02 - 0.62 µg L^{-1}	0.01 µg L^{-1}	Canada	Muir and Baker 1976
	deethylatrazine	cyprazine	0.15 - 3.6 µg L^{-1}	0.01 µg L^{-1}	Canada	Muir and Baker 1976
	metolachlor ethane sulfonic acid	metolachlor	5 - > 20 µg L^{-1}	0.2 µg L^{-1}	USA	Phillips et al. 1999
	metolachlor oxanilic acid	metolachlor	1 - 10 µg L^{-1}	0.2 µg L^{-1}	USA	Phillips et al. 2002
ditch						
	2,4-D methyl ester	2,4-D	ND	<0.19 µg L^{-1}	USA	Battaglin et al. 2009
	2-isoprpyl-6-methyl-4-hydroxypyrimidine	diazinon	ND	1 µg L^{-1}	Canada	Li et al. 2002
	diazoxon	diazinon	ND	0.03 µg L^{-1}	Canada	Li et al. 2002
	deisopropylatrazine	atrazine, cyanazine and simazine	0.17 µg L^{-1}	0.08 µg L^{-1}	USA	Battaglin et al. 2009
	hydroxyatrazine	atrazine	0.682 µg L^{-1}	-	USA	Battaglin et al. 2009
	diaminochlorotriazine	atrazine	0.062 µg L^{-1}	0.04 µg L^{-1}	USA	Battaglin et al. 2009
	aminomethylphosphonic acid	glyphosate	2.9 µg L^{-1}	0.02 µg L^{-1}	USA	Battaglin et al. 2009
stream						
	acetochlor ethane sulfonic acid	acetochlor	< 0.2 - 1.6 µg L^{-1}	0.2 µg L^{-1}	USA	Kalkhoff et al. 2003
	acetochlor oxanilic acid	acetochlor	< 0.02 - 1.4 µg L^{-1}	0.2 µg L^{-1}	USA	Kalkhoff et al. 2003
	2,6-diethylanaline	alachlor	ND	0.01 µg L^{-1}	USA	Hoffman et al. 2000
	alachlor ethane sulfonic acid	alachlor	< 0.2 - 3.5 µg L^{-1}	0.2 µg L^{-1}	USA	Kalkhoff et al. 2003
	alachlor ethane sulfonic acid	alachlor	0.8 - 5.2 µg L^{-1} [c]	0.1 µg L^{-1}	USA	Kolpin et al. 1996a
			5.2 - 27.8 µg L^{-1} [b]	0.1 µg L^{-1}	USA	Kolpin et al. 1996a
	alachlor oxanilic acid	alachlor	< 0.2 - 0.54 µg L^{-1}	0.2 µg L^{-1}	USA	Kalkhoff et al. 2003
	aldicarb sulfone	aldicarb	ND	0.05 µg L^{-1}	USA	Hoffman et al. 2000
	aldicarb sulfoxide	aldicarb	ND	0.05 µg L^{-1}	USA	Hoffman et al. 2000
	deethylatrazine	atrazine and propazine	< 0.05 - 0.39 µg L^{-1}	0.05 µg L^{-1}	USA	Kalkhoff et al. 2003
			0.04 µg L^{-1} [b]	0.01 µg L^{-1}	USA	Hoffman et al. 2000
			23 µg L^{-1} [b]	0.05 µg L^{-1}	USA	Lerch et al. 1995
			0.04 µg L^{-1}	0.03 µg L^{-1}	USA	Battaglin et al. 2009
	deisopropylatrazine	atrazine, cyanazine and simazine	< 0.05 - 0.36 µg L^{-1}	0.05 µg L^{-1}	USA	Kalkhoff et al. 2003

Table A4. The occurrence of pesticide transformation products in environmental systems (Chapter 2)

Environmental compartment	Transformation product	Parent pesticide [a]	Concentration	Limit of detection	Country	Reference
stream continued...			ND	0.08 µg L^{-1}	USA	Battaglin et al. 2009
	hydroxyatrazine	atrazine	< 0.2 - 8.8 µg L^{-1}	0.2 µg L^{-1}	USA	Kalkhoff et al. 2003
			0.18 - 5.7 µg L^{-1}	0.04 µg L^{-1}	USA	Lerch et al. 1995
			ND	0.032 µg L^{-1}	USA	Battaglin et al. 2009
	deethyl hydroxyatrazine	atrazine	<0.12 - 1.9 µg L^{-1}	0.12 µg L^{-1}	USA	Lerch et al. 1995
	deisopropyl hydroxyatrazine	atrazine	<0.12 - 0.72 µg L^{-1}	0.12 µg L^{-1}	USA	Lerch et al. 1995
	diaminochlorotriazine	atrazine	ND	0.04 µg L^{-1}	USA	Battaglin et al. 2009
	cyanazine amide	cyanazine	< 0.05 - 1.2 µg L^{-1}	0.05 µg L^{-1}	USA	Kalkhoff et al. 2003
	3-hydroxycarbofuran	carbofuran	ND	0.05 µg L^{-1}	USA	Hoffman et al. 2000
	2,4-D methyl ester	2,4-D	ND	<0.016 µg L^{-1}	USA	Battaglin et al. 2009
	p,p'-DDE	DDT	ND	0.01µg L^{-1}	USA	Hoffman et al. 2000
	alpha-HCH	gamma-HCH	ND	0.01 µg L^{-1}	USA	Hoffman et al. 2000
	aminomethylphosphonic acid	glyphosate	0.21 µg L^{-1}	0.02 µg L^{-1}	USA	Battaglin et al. 2009
	metolachlor ethane sulfonic acid	metolachlor	< 0.2 - 6.7 µg L^{-1}	0.2 µg L^{-1}	USA	Kalkhoff et al. 2003
			< 0.2 - 0.57 µg L^{-1}	0.2 µg L^{-1}	USA	Phillips et al. 1999
	metolachlor oxanilic acid	metolachlor	< 0.2 - 1.3 µg L^{-1}	0.2 µg L^{-1}	USA	Kalkhoff et al. 2003
			< 0.2 - > 0.5 µg L^{-1}	0.2 µg L^{-1}	USA	Phillips et al. 1999
	trifluoromethylphenyl urea	fluometuron	ND	0.05 µg L^{-1}	USA	Coupe et al. 1998
	deisopropylprometryn	prometryn	ND	0.05 µg L^{-1}	USA	Coupe et al. 1998
	3,4-dichloroaniline	propanil	0.9 µg L^{-1}	0.05 µg L^{-1}	USA	Coupe et al. 1998
	methomyl	thiodicarb	0.09 ppb	0.04 ppb	USA	EPA 1998k
	triclopyr	triclopyr triethylamine salt	0.64 ppm (sediment)	post-treatment	USA	EPA 1998l
	3,5,6-trichloro-2-pyridinol	triclopyr triethylamine salt	0.06 - 0.18 ppm	1 - 8 hours	USA	EPA 1998l
river						
	2,4-dichlorophenol	2,4-D	ND	75 ng L^{-1}	Italy	Lagana et al. 2002
	2,4-D methyl ester	2,4-D	ND	<0.19 µg L^{-1}	USA	Battaglin et al. 2009
	acetochlor oxanilic acid	acetochlor	ND - 0.15 µg L^{-1}	0.01 µg L^{-1}	USA	Ferrer et al. 1997
	alachlor ethane sulfonic acid	alachlor	1.55 - 4.75 µg L^{-1} [c]	0.1 µg L^{-1}	USA	Battaglin and Goolsby 1999
			2.1 µg L^{-1}	0.05 µg L^{-1}	USA	Verstraeten et al. 1999
	alachlor oxanilic acid	alachlor	ND - 0.21 µg L^{-1}	0.01 µg L^{-1}	USA	Ferrer et al. 1997

Table A4. The occurrence of pesticide transformation products in environmental systems (Chapter 2)

Environmental compartment	Transformation product	Parent pesticide [a]	Concentration	Limit of detection	Country	Reference
river continued...	2,6-diethylaniline	alachlor	ND - 0.924 µg L^{-1}	5 ng L^{-1}	USA	Pereira and Rostad 1990
	2-chloro-2',6'-diethylacetanilide	alachlor	ND - 0.35 µg L^{-1}	5 ng L^{-1}	USA	Pereira and Rostad 1990
	2-hydroxy-2',6'-diethylacetanilide	alachlor	ND - 0.9 µg L^{-1}	5 ng L^{-1}	USA	Pereira and Rostad 1990
	8-hydroxy-bentazone	bentazone	ND - 27 µg L^{-1}	2 ng L^{-1}	Italy	Lagana et al. 2002
	cyanazine amide	cyanazine	0.47 - 0.57 µg L^{-1} [c]	0.05 µg L^{-1}	USA	Battaglin and Goolsby 1999
			0.06 µg L^{-1} [c]	0.02 µg L^{-1}	USA	Lerch and Blanchard 2003
			ND - 222 ng L^{-1}	25 ng L^{-1}	USA	Pereira and Hostettler 1993
	deethylcyanazine	cyanazine	< 0.05 µg L^{-1} [c]	0.05 µg L^{-1}	USA	Battaglin and Goolsby 1999
			ND	0.05 µg L^{-1}	USA	Verstraeten et al. 1999
	deethylcyanazine amide	cyanazine	< 0.05 µg L^{-1} [c]	0.5 µg L^{-1}	USA	Battaglin and Goolsby 1999
	deethylatrazine	atrazine and propazine	0.42 - 0.47 µg L^{-1} [c]	0.05 µg L^{-1}	USA	Battaglin and Goolsby 1999
			0.39 - 4.4 µg L^{-1} [b]	0.05 µg L^{-1}	USA	Thurman et al. 1992
			ND - 0.407 µg L^{-1}	0.005 µg L^{-1}	Greece	Albanis et al. 1998
			ND - 0.215 µg L^{-1}	0.01 µg L^{-1}	Greece	Albanis and Hela 1998
			0.025 - 0.08 µg L^{-1}	0.3 ng L^{-1}	USA	Sabik et al. 2003
			7 - 82 ng L^{-1}	5 ng L^{-1}	USA	Pereira and Rostad 1990
			5 - 855 ng L^{-1}	5 ng L^{-1}	USA	Pereira and Hostettler 1993
			150 ng L^{-1} [b]	1 ng L^{-1}	USA	Liu et al. 2002
			12 - 28 µg L^{-1} [c]	-	USA	Solomon et al. 1996
			ND	0.028 µg L^{-1}	USA	Battaglin et al. 2009
			1.7 µg L^{-1} [b]	0.05 µg L^{-}	Canada	Struger and Fletcher 2007
	deisopropylatrazine	atrazine, cyanazine and simazine	0.43 - 0.87 µg L^{-1} [c]	0.05 µg L^{-1}	USA	Battaglin and Goolsby 1999
			< 0.05 - 3.2 µg L^{-1} [b]	0.05 µg L^{-1}	USA	Thurman et al. 1992
			0.007 - 0.038 µg L^{-1}	0.3 ng L^{-1}	USA	Sabik et al. 2003

Table A4. The occurrence of pesticide transformation products in environmental systems (Chapter 2)

Environmental compartment	Transformation product	Parent pesticide [a]	Concentration	Limit of detection	Country	Reference
river continued...			8 - 45 ng L^{-1}	5 ng L^{-1}		Pereira and Rostad 1990
			ND - 335 ng L^{-1}	10 ng L^{-1}	USA	Pereira and Hostettler 1993
			64 ng L^{-1} [b]	1.8 ng L^{-1}	USA	Liu et al. 2002
			4.9 - 15 µg L^{-1} [c]	-	USA	Solomon et al. 1996
			ND	0.08 µg L^{-1}	USA	Battaglin et al. 2009
	hydroxyatrazine	atrazine	ND	0.032 µg L^{-1}	USA	Battaglin et al. 2009
	diaminochlorotriazine	atrazine	ND	0.04 µg L^{-1}	USA	Battaglin et al. 2009
	p,p'-DDE	DDT	4 ng L^{-1} [b]	0.3 ng L^{-1}	USA	Liu et al. 2002
	dimethenamid ethane sulfonic acid	dimethenamid	0.05 µg L^{-1} [c]	0.03 µg L^{-1}	USA	Zimmerman et al. 2002
	dimethenamid oxanilic acid	dimethenamid	0.05 µg L^{-1} [c]	0.02 µg L^{-1}	USA	Zimmerman et al. 2002
	endosulfan sulphate	endosulfan	6 ng L^{-1}	0.3 ng L^{-1}	USA	Liu et al. 2002
	flufenacet ethane sulfonic acid	flufenacet	0.06 µg L^{-1} [c]	0.01 µg L^{-1}	USA	Zimmerman et al. 2002
	flufenacet oxanilic acid	flufenacet	0.05 µg L^{-1} [c]	0.07 µg L^{-1}	USA	Zimmerman et al. 2002
	aminomethylphosphonic acid	glyphosate	ND	0.02 µg L^{-1}	USA	Battaglin et al. 2009
	4-chloro-2-methylphenol	MCPA	ND	50 ng L^{-1}	Italy	Lagana et al. 2002
	metolachlor oxanilic acid	metolachlor	ND - 0.29 µg L^{-1}	0.01 µg L^{-1}	USA	Ferrer et al. 1997
	metolachlor ethane sulfonic acid	metolachlor	0.33 - 1.82 µg L^{-1}	0.01 µg L^{-1}	USA	Ferrer et al. 1997
	3,4-dichloroaniline	propanil	ND - 26 ppb	0.05 ppb	USA	PSD 1988a
canal						
	deethylatrazine	atrazine	ND - 0.526	0.01 µg L^{-1}	Greece	Albanis and Hela 1998
			0.03 µg L^{-1}	-	USA	Battaglin et al. 2009
	deisopropylatrazine	atrazine, cyanazine and simazine	ND	0.08 µg L^{-1}	USA	Battaglin et al. 2009
	2,4-D methyl ester	2,4-D	ND	0.016 µg L^{-1}	USA	Battaglin et al. 2009
	aminomethylphosphonic acid	glyphosate	ND	0.02 µg L^{-1}	USA	Battaglin et al. 2009
	diaminochlorotriazine	atrazine	ND	0.04 µg L^{-1}	USA	Battaglin et al. 2009
pond						
	2,4-D methyl ester	2,4-D	ND	0.19 µg L^{-1}	USA	Battaglin et al. 2009

Table A4. The occurrence of pesticide transformation products in environmental systems (Chapter 2)

Environmental compartment	Transformation product	Parent pesticide [a]	Concentration	Limit of detection	Country	Reference
pond continued...	deethylatrazine	atrazine	0.022 µg L^{-1}	-	USA	Battaglin et al. 2009
	deisopropylatrazine	atrazine, cyanazine and simazine	ND	0.08 µg L^{-1}	USA	Battaglin et al. 2009
	hydroxyatrazine	atrazine	0.263 µg L^{-1}	0.032 µg L^{-1}	USA	Battaglin et al. 2009
	diaminochlorotriazine	atrazine	ND	0.04 µg L^{-1}	USA	Battaglin et al. 2009
	aminomethylphosphonic acid	glyphosate	ND	0.02 µg L^{-1}	USA	Battaglin et al. 2009
lake						
	deethylatrazine	atrazine	1.57 µg L^{-1} [b]	0.05 µg L^{-1}	USA	Spalding et al. 1994
			92 ng L^{-1} [c]	2 - 6 ng L^{-1}	Switzerland	Bucheli et al. 1997
			0.36 µg L^{-1} [c]	0.05 µg L^{-1}	USA	Thurman et al. 2000
			0.18 - 1.57 µg L^{-1} [b] 0.1 - 0.54 µg L^{-1} [c]	0.05 µg L^{-1}	USA	Spalding et al. 1994
	deisopropylatrazine	atrazine	1.06 µg L^{-1} [b]	0.09 µg L^{-1}	USA	Spalding et al. 1994
			26 ng L^{-1} [c]	2 - 6 ng L^{-1}	Switzerland	Bucheli et al. 1997
			ND - 1.06 µg L^{-1} [b] ND - 0.92 µg L^{-1} [c]	0.09 µg L^{-1}	USA	Spalding et al. 1994
	hydroxyatrazine	atrazine	0.56 µg L^{-1} [c]	0.05 µg L^{-1}	USA	Thurman et al. 2000
	dichlorophenylurea	diuron	0.2 µg L^{-1} [c]	0.2 µg L^{-1}	USA	Thurman et al. 2000
	dichloromethylphenylurea	diuron	0.45 µg L^{-1} [c]	0.2 µg L^{-1}	USA	Thurman et al. 2000
	3,4-dichloroaniline	diuron	0.31 µg L^{-1} [c]	0.05 µg L^{-1}	USA	Thurman et al. 2000
	metolachlor ethane sulfonic acid	metolachlor	0.1 µg L^{-1} [c]	0.2 µg L^{-1}	USA	Thurman et al. 2000
	metolachlor oxanilic acid	metolachlor	0.19 µg L^{-1} [c]	0.2 µg L^{-1}	USA	Thurman et al. 2000
	demethylnorflurazon	norflurazon	0.17 µg L^{-1} [c]	0.05 µg L^{-1}	USA	Thurman et al. 2000
Groundwater						
	3-chloroallyl alcohol	1,3-dichloropropene	trace - 13.5 ppb	0.05 ppb	USA	EPA 1998a
	3-chloroacrylic acid	1,3-dichloropropene	trace - 8.79 ppb	0.05 ppb	USA	EPA 1998a
	2,4-dichlorophenol	2,4-D	4 µg L^{-1} [b]	-	Denmark	Helweg et al. 2002
	acetochlor ethane sulfonic acid	acetochlor	0.77 µg L^{-1} [b]	0.2 µg L^{-1}	USA	Kolpin et al. 2000
			ND - 3.32 µg L^{-1}	0.2 µg L^{-1}	USA	Boyd 2000
	acetochlor ethane sulfonic acid	acetochlor	0.28 µg L^{-1} [c]	0.1 µg L^{-1}	USA	Kolpin et al. 1996a

Table A4. The occurrence of pesticide transformation products in environmental systems (Chapter 2)

Environmental compartment	Transformation product	Parent pesticide [a]	Concentration	Limit of detection	Country	Reference
Groundwater continued...			8.6 µg L^{-1} [b]	0.1 µg L^{-1}	USA	Kolpin et al. 1996a
	acetochlor oxanilic acid	acetochlor	11.5 µg L^{-1} [b]	0.2 µg L^{-1}	USA	Kolpin et al. 2000
			ND - 1.75 µg L^{-1}	0.2 µg L^{-1}	USA	Boyd 2000
			ND - 0.17 µg L^{-1}	0.01 µg L^{-1}	USA	Ferrer et al. 1997
	α-N-[(2'-6'-diethylphenylamino)ethanol	alachlor	< 2 - 480 ng L^{-1}	-	USA	Potter and Carpenter 1995
	2-chloro-2'-ethyl-6'-ethyl-N-(methoxymethyl)acetanilide	alachlor	< 2 - 310 ng L^{-1}	-	USA	Potter and Carpenter 1995
	2'-acetyl-6'-ethylacetanilide	alachlor	28 - 120 ng L^{-1}	-	USA	Potter and Carpenter 1995
	2'-acetyl-6'-ethyl-N-methoxymethyl)acetanilide	alachlor	68 - 240 ng L^{-1}	-	USA	Potter and Carpenter 1995
	2-hydroxy-2',6'-diethyl-N-methyl)acetanilide	alachlor	< 2 - 130 ng L^{-1}	-	USA	Potter and Carpenter 1995
	2-hydroxy-2',6'-diethyl-N-methoxymethyl)acetanilide	alachlor	< 2 - 100 ng L^{-1}	-	USA	Potter and Carpenter 1995
	2,6-diethylaniline	alachlor	0.085 µg L^{-1} [b]	0.003 µg L^{-1}	USA	Kolpin et al. 1998
			< 2 - 16 ng L^{-1}	-	USA	Potter and Carpenter 1995
			0.02 µg L^{-1} [b]	0.02 µg L^{-1}	USA	Kolpin et al. 1996b
	2',6'-diethylacetanilide	alachlor	< 2 - 130 ng L^{-1}	-	USA	Potter and Carpenter 1995
	2',6'-diethylformanilide	alachlor	< 2 - 87 ng L^{-1}	-	USA	Potter and Carpenter 1995
	7-ethylindoline	alachlor	< 2 - 35 ng L^{-1}	-	USA	Potter and Carpenter 1995
	alachlor ethane sulfonic acid	alachlor	1.2 µg L^{-1} [b]	0.05 µg L^{-1}	USA	Verstraeten et al. 1999
			8.63 µg L^{-1} [b]	0.1 µg L^{-1}	USA	Kolpin et al. 1996b
			8.5 µg L^{-1} [b]	0.2 µg L^{-1}	USA	Kolpin et al. 2000
			ND - 2.5 µg L^{-1}	0.2 µg L^{-1}	USA	Boyd 2000
			0.06 - 9.32 µg L^{-1}	0.05 µg L^{-1}	USA	Aga et al. 1994
			0.21 - 6.91 µg L^{-1}	-	USA	EPA 1998b
	alachlor oxanilic acid	alachlor	33.4 µg L^{-1} [b]	0.2 µg L^{-1}	USA	Kolpin et al. 2000
			ND - 0.31 µg L^{-1}	0.2 µg L^{-1}	USA	Boyd 2000
			0.02 - 1.66 µg L^{-1}	0.01 µg L^{-1}	USA	Ferrer et al. 1997

Table A4. The occurrence of pesticide transformation products in environmental systems (Chapter 2)

Environmental compartment	Transformation product	Parent pesticide [a]	Concentration	Limit of detection	Country	Reference
Groundwater continued...	N-(2,6-diethylphenyl) methylene	alachlor	< 2 - 10 ng L^{-1}	-	USA	Potter and Carpenter 1995
	N-(2,6-diethylphenyl)-N-(methoxymethyl)acetamide	alachlor	100 - 550 ng L^{-1}	-	USA	Potter and Carpenter 1995
	deethylatrazine	atrazine	0.205 µg L^{-1} [b]	1 - 5 ng L^{-1}	Greece	Albanis et al. 1998
			0.4 µg L^{-1} [c]	0.04 µg L^{-1}	USA	Steinheimer and Scoggin 2001
			2.32 µg L^{-1} [b]	0.05 µg L^{-1}	USA	Burkart and Kolpin 1993
			7 ng L^{-1}	-	Switzerland	Bucheli et al. 1997
			2.6 µg L^{-1} [b]	0.002 µg L^{-1}	USA	Kolpin et al. 1998
			5 µg L^{-1}	0.02 µg L^{-1}	USA	Adams and Thurman 1991
			2.2 µg L^{-1} [b]	0.05 µg L^{-1}	USA	Kolpin et al. 1996b
			0.59 µg L^{-1} [b]	0.05 µg L^{-1}	USA	Kolpin et al. 2000
			ND - 0.44 µg L^{-1}	0.05 µg L^{-1}	USA	Boyd 2000
			0.05 - 0.13 µg L^{-1} [b]	0.02 µg L^{-1}	USA	Blanchard and Donald 1997
			0.42 µg L^{-1}	-	Australia	APVMA 1997a
			1.86 µg L^{-1}	0.05 µg L^{-1}	France	Baran et al. 2008
			1.16 µg L^{-1} [b]	0.05 µg L^{-1}	France	Baran et al. 2007
			1.03 µg L^{-1}	-	USA	Steele et al. 2008
	deisopropylatrazine	atrazine, cyanazine, simazine	0.6 µg L^{-1} [c]	0.04 µg L^{-1}	USA	Steinheimer and Scoggin 2001
			0.16 µg L^{-1}	-	Australia	APVMA 1997a
			1.17 µg L^{-1} [b]	0.05 µg L^{-1}	USA	Kolpin et al. 1996b
			14 ng L^{-1}	-	Switzerland	Bucheli et al. 1997
			< 0.02 µg L^{-1}	0.02 µg L^{-1}	USA	Adams and Thurman 1991
			1.1 µg L^{-1} [b]	0.05 µg L^{-1}	USA	Kolpin et al. 2000
			ND - 0.26 µg L^{-1}	0.05 µg L^{-1}	USA	Boyd 2000
			0.36 µg L^{-1} [b]	-	Spain	Hernandez et al. 2008
	deisopropylhydroxyatrazine	atrazine, cyanazine, simazine	0.04 µg L^{-1} [c]	0.04 µg L^{-1}	USA	Steinheimer and Scoggin 2001
	hydroxyatrazine	atrazine	1.3 µg L^{-1} [b]	0.2 µg L^{-1}	USA	Kolpin et al. 2000

Table A4. The occurrence of pesticide transformation products in environmental systems (Chapter 2)

Environmental compartment	Transformation product	Parent pesticide [a]	Concentration	Limit of detection	Country	Reference
Groundwater continued...			ND - 0.22 µg L^{-1}	0.2 µg L^{-1}	USA	Boyd 2000
	2-aminobenzimidazole	carbendazim [a]	0.03 µg L^{-1} [b]	-	Spain	Hernandez et al. 2008
	3-hydroxy carbofuran	carbofuran	ND	-	Spain	Hernandez et al. 2008
	carbofuran-7-PhOH-3CO	carbofuran	0.06	-	Spain	Hernandez et al. 2008
	3-carbamyl-1,2,4,5-trichlorobenzoic acid, 3-cyano-6-hydroxy-2,4,5-trichlorobenzamide, 4-hydroxy-2,5,6-trichloroisophthalonitrile and 3-cyano-2,4,5,6-tetrachlorobenzamide combined	chlorothalonil	16 µg L^{-1}	1.5 µg L^{-1}	USA	EPA 1999b
	3-carbamyl-2,4,5-trichlorobenzoic acid	chlorothalonil	trace - 10.1 µg L^{-1}	1.5 µg L^{-1}	USA	EPA 1999b
			2 - 12.6 µg L^{-1}	2 µg L^{-1}	USA	EPA 1999b
			<0.1 - 10.1 µg L^{-1}	-	USA	EU 2005b
			1.8 - 10.1 µg L^{-1}	-	USA	EPA 1999b
	3-cyano-6-hydroxy-2,4,5-trichlorobenzamide	chlorothalonil	0.2 µg L^{-1}	1.5 µg L^{-1}	USA	EPA 1999b
			2 - 5 µg L^{-1}	2 µg L^{-1}	USA	EPA 1999b
			<0.2 - 0.2 µg L^{-1}	-		EPA 1999b
	3-cyano-2,5,6-trichlorobenzamide	chlorothalonil	ND	1.5 µg L^{-1}	USA	EPA 1999b
	4-hydroxy-2,5,6-trichloroisophthalonitrile	chlorothalonil	3.6 µg L^{-1}	2 µg L^{-1}	USA	EPA 1999b
	3-cyano-2,4,5,6-tetrachlorobenzamide	chlorothalonil	2.8 µg L^{-1}	2 µg L^{-1}	USA	EPA 1999b
	3,4-dichloroaniline	chlorpyrifos, diuron, linuron, propanil	<0.025 µg L^{-1} [b]	-	Spain	Hernandez et al. 2008
	cyanazine amide	cyanazine	0.55 µg L^{-1} [b]	0.55 µg L^{-1}	USA	Kolpin et al. 1996b
			0.64 µg L^{-1} [b]	0.05 µg L^{-1}	USA	Kolpin et al. 2000
			ND - 0.31 µg L^{-1}	0.05 µg L^{-1}	USA	Boyd 2000
	deethylcyanazine	cyanazine	ND	0.05 µg L^{-1}	USA	Verstraeten et al. 1999
			ND	0.05 µg L^{-1}	USA	Kolpin et al. 1996b
	deethylcyanazine amide	cyanazine	ND	0.05 µg L^{-1}	USA	Kolpin et al. 1996b
	3,5,6-trichloro-2-pyridinol	chlorpyrifos	ND	50 µg L^{-1}	USA	EPA 1999d
	2-methoxy-3,5,6-trichloropyridine	chlorpyrifos	ND	10 µg L^{-1}	USA	EPA 1999d
	chlorthal-dimethyl mono-acid and di-acid	chlorthal-dimethyl	ND - 158.2 µg L^{-1} [a]	0.05 µg L^{-1}	USA	Monohan et al. 1995

Table A4. The occurrence of pesticide transformation products in environmental systems (Chapter 2)

Environmental compartment	Transformation product	Parent pesticide [a]	Concentration	Limit of detection	Country	Reference
Groundwater continued...	chlorthal-dimethyl di-acid	chlorthal-dimethyl	2.22 µg L^{-1} [b]	0.01 µg L^{-1}	USA	Kolpin et al. 1996b
	p,p'-DDE	DDT	0.006 µg L^{-1} [b]	0.006 µg L^{-1}	USA	Kolpin et al. 1998
			0.03 µg L^{-1} [b]	0.03 µg L^{-1}	-	Kolpin et al. 1996b
	2,6-dichlorbenzamide	diclobenil	180 ppb	-	Netherlands	EPA 1998e
	4-chloroaniline	diflubenzuron	ND	-	Spain	Hernandez et al. 2008
	endosulfan sulphate	endosulfan	ND - 1.4 ppb	0.005 ppb	USA	EPA 2002c
	AMPA	glyphosate	1.6 µg L^{-1} [b]	-	Denmark	Helweg et al. 2002
	α-HCH	gamma-HCH	0.059 µg L^{-1} [b]	0.002 µg L^{-1}	USA	Kolpin et al. 1998
	monodesmethyl isoproturon	isoproturon	~0.05 µg L^{-1}	≤ 0.05 µg L^{-1}	France	Baran et al. 2008
	didesmethylisoproturon	isoproturon	ND	≤ 0.05 µg L^{-1}	France	Baran et al. 2008
	metolachlor ethane sulfonic acid	metolachlor	8.6 µg L^{-1} [b]	0.2 µg L^{-1}	USA	Kolpin et al. 2000
			ND - 6.84 µg L^{-1}	0.2 µg L^{-1}	USA	Boyd 2000
			0.1 - 1.83 µg L^{-1}	0.01 µg L^{-1}	USA	Ferrer et al. 1997
			15.2 µg L^{-1}	-	USA	Steele et al. 2008
	metolachlor oxanilic acid	metolachlor	15.3 µg L^{-1} [b]	0.2 µg L^{-1}	USA	Kolpin et al. 2000
			ND - 4.25 µg L^{-1}	0.2 µg L^{-1}	USA	Boyd 2000
			0.03 - 0.91 µg L^{-1}	0.01 µg L^{-1}	USA	Ferrer et al. 1997
	2,4-bis(isopropylamino)-6-hydroxy-s-triazine	prometryn	0.61 ppb	-	USA	EPA 1996g
	hydroxysimazine	simazine	0.15 µg L^{-1} [c]	0.04 µg L^{-1}	USA	Steinheimer and Scoggin 2001
	desethyl-2-hydroxyterbuthylazine	terbuthylazine	0.21 µg L^{-1} [b]	-	Spain	Hernandez et al. 2008
	desethylterbuthylazine	terbuthylazine	1.42 µg L^{-1} [b]	-	Spain	Hernandez et al. 2008
	hydroxyterbuthylazine	terbuthylazine	0.15 µg L^{-1} [b]	-	Spain	Hernandez et al. 2008
	desethylterbumeton	terbumeton	1.62 µg L^{-1} [b]	-	Spain	Hernandez et al. 2008
	methomyl	thiodicarb	0.1 -0.4 ppb	-	USA	EPA 1998k
Raw source water	hydroxyacetochlor	acetochlor	198 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006

Table A4. The occurrence of pesticide transformation products in environmental systems (Chapter 2)

Environmental compartment	Transformation product	Parent pesticide [a]	Concentration	Limit of detection	Country	Reference
Raw source water continued...	deschloroacetochlor	acetochlor	35 ng L^{-1} [b]	0.07 ng L^{-1}	USA	Hladik et al. 2006
	acetochlor oxanilic acid	acetochlor	1170 ng L^{-1} [b]	7 ng L^{-1}	USA	Hladik et al. 2006
	acetochlor ethane sulfonic acid	acetochlor	1080 ng L^{-1} [b]	100 ng L^{-1}	USA	Hladik et al. 2006
	2-chloro-2'-ethyl-6'-methylacetanilide	acetochlor	167 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
	2-hydroxy-2'-ethyl-6'-methylacetanilide	acetochlor	105 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
	2-ethyl-6-methylaniline	acetochlor	<25 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
	2'-ethyl-6'-methylacetanilide	acetochlor	57 ng L^{-1} [b]	8 ng L^{-1}	USA	Hladik et al. 2006
	hydroxyalachlor	alachlor	43 ng L^{-1} [b]	3 ng L^{-1}	USA	Hladik et al. 2006
	deschloroalachlor	alachlor	14 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
	2-chloro-2'-6'-diethylacetanilide	alachlor	15 ng L^{-1} [b]	0.1 ng L^{-1}	USA	Hladik et al. 2006
	2-hydroxy-2'-6'-diethylacetanilide	alachlor	104 ng L^{-1} [b]	0.7 ng L^{-1}	USA	Hladik et al. 2006
	2-hydroxy-2'-6'-diethyl-N-methylacetanilide	alachlor	1.7 ng L^{-1} [b]	4 ng L^{-1}	USA	Hladik et al. 2006
	2'-6'-diethylacetanilide	alachlor	43 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
	2,6-diethylaniline	alachlor	<11 ng L^{-1} [b]	10 ng L^{-1}	USA	Hladik et al. 2006
	alachlor oxanilic acid	alachlor	216 ng L^{-1} [b]	7 ng L^{-1}	USA	Hladik et al. 2006
	alachlor ethane sulfonic acid	alachlor	945 ng L^{-1} [b]	100 ng L^{-1}	USA	Hladik et al. 2006
	deethylatrazine	atrazine	0.14 - 0.24 µg L^{-1} [c]	-	USA	Solomon et al. 1996
			0.38 µg L^{-1} [c]	-	USA	Solomon et al. 1996
			0.682 µg L^{-1} [b]	-	USA	Coupe and Blomquist 2004
	deethylatrazine continued	atrazine	594 ng L^{-1} [b]	0.3 ng L^{-1}	USA	Hladik et al. 2006
	deisopropylatrazine	atrazine	0.08 - 0.14 µg L^{-1} [c]	-	USA	Solomon et al. 1996
			0.1 µg L^{-1} [c]	-	USA	Solomon et al. 1996
			199 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
	hydroxyatrazine	atrazine	0.8 µg L^{-1} [c]	-	USA	Solomon et al. 1996
	azinphos-methyl-oxon	azinphos-methyl	0.263 µg L^{-1} [c]	0.031 µg L^{-1}	USA	Nguyen et al. 2004
	o-p'-DDA	DDT	0.28 µg L^{-1}	-	Germany	Heberer and Dünnbier 1999
	p-p'-DDA	DDT	1.7 µg L^{-1}	-	Germany	Heberer and Dünnbier 1999
	deschlorodimethenamid	dimethenamid	14 ng L^{-1} [b]	0.1 ng L^{-1}	USA	Hladik et al. 2006

Table A4. The occurrence of pesticide transformation products in environmental systems (Chapter 2)

Environmental compartment	Transformation product	Parent pesticide [a]	Concentration	Limit of detection	Country	Reference
Raw source water continued...	disulfoton sulfone	disulfoton	0.013 µ g L^{-1} [c]	0.005 µg L^{-1}	USA	Nguyen et al. 2004
	disulfoton sulfoxide	disulfoton	0.06 µg L^{-1} [c]	0.016 µg L^{-1}	USA	Nguyen et al. 2004
	fenamiphos sulfone	fenamiphos	0.005 µg L^{-1} [c]	0.008 µg L^{-1}	USA	Nguyen et al. 2004
	fenamiphos sulfoxide	fenamiphos	0.021 µg L^{-1} [c]	0.008 µg L^{-1}	USA	Nguyen et al. 2004
	malaoxon	malathion	ND	0.005 µg L^{-1}	USA	Nguyen et al. 2004
	hydroxymetolachlor	metolachlor	217 ng L^{-1} [b]	1 ng L^{-1}	USA	Hladik et al. 2006
	deschlorometolachlor	metolachlor	32 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
	metolachlor morpholinone	metolachlor	63 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
	metolachlor propanol	metolachlor	208 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
	deschloroacetylmetachlor	metolachlor	39 ng L^{-1} [b]	0.1 ng L^{-1}	USA	Hladik et al. 2006
	deschloroacetyl metachlor propanol	metolachlor	17 ng L^{-1} [b]	0.8 ng L^{-1}	USA	Hladik et al. 2006
	metachlor oxanilic acid	metolachlor	687 ng L^{-1} [b]	7 ng L^{-1}	USA	Hladik et al. 2006
	metachlor ethane sulfonic acid	metolachlor	1580 ng L^{-1} [b]	90 ng L^{-1}	USA	Hladik et al. 2006
Finished drinking water						
	hydroxyacetochlor	acetochlor	64 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
	deschloroacetochlor	acetochlor	31 ng L^{-1} [b]	0.07 ng L^{-1}	USA	Hladik et al. 2006
	acetochlor oxanilic acid	acetochlor	551 ng L^{-1} [b]	7 ng L^{-1}	USA	Hladik et al. 2006
	acetochlor ethane sulfonic acid	acetochlor	845 ng L^{-1} [b]	100 ng L^{-1}	USA	Hladik et al. 2006
	2-chloro-2'-ethyl-6'-methylacetanilide	acetochlor	163 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
	2-hydroxy-2'-ethyl-6'-methylacetanilide	acetochlor	67 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
	2-ethyl-6-methylaniline	acetochlor	<25 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
	2'-ethyl-6'-methylacetanilide	acetochlor	57 ng L^{-1} [b]	8 ng L^{-1}	USA	Hladik et al. 2006
	hydroxyalachlor	alachlor	34 ng L^{-1} [b]	3 ng L^{-1}	USA	Hladik et al. 2006
	deschloroalachlor	alachlor	0.7 ng L^{-1} [b]	-	USA	Hladik et al. 2006
	2-chloro-2'-6'-diethylacetanilide	alachlor	11 ng L^{-1} [b]	0.1 ng L^{-1}	USA	Hladik et al. 2006
	2-hydroxy-2'-6'-diethylacetanilide	alachlor	85 ng L^{-1} [b]	0.7 ng L^{-1}	USA	Hladik et al. 2006
	2-hydroxy-2'-6'-diethyl-N-methylacetanilide	alachlor	1.7 ng L^{-1} [b]	4 ng L^{-1}	USA	Hladik et al. 2006
	2'-6'-diethylacetanilide	alachlor	38 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
	2,6-diethylaniline	alachlor	<11 ng L^{-1} [b]	10 ng L^{-1}	USA	Hladik et al. 2006

Table A4. The occurrence of pesticide transformation products in environmental systems (Chapter 2)

Environmental compartment	Transformation product	Parent pesticide [a]	Concentration	Limit of detection	Country	Reference
Finished drinking water continued...	alachlor oxanilic acid	alachlor	136 ng L^{-1} [b]	7 ng L^{-1}	USA	Hladik et al. 2006
	alachlor ethane sulfonic acid	alachlor	743 ng L^{-1} [b]	100 ng L^{-1}	USA	Hladik et al. 2006
	deethylatrazine	atrazine	318 ng L^{-1} [b]	0.3 ng L^{-1}	USA	Hladik et al. 2006
			0.352 µg L^{-1} [b]	-	USA	Coupe and Blomquist 2004
	deisopropylatrazine	atrazine	75 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
	azinphos-methyl-oxon	azinphos-methyl	0.026 µg L^{-1} [c]	0.031 µg L^{-1}	USA	Nguyen et al. 2004
	deschlorodimethenamid	dimethenamid	25 ng L^{-1} [b]	0.1 ng L^{-1}	USA	Hladik et al. 2006
	disulfoton sulfone	disulfoton	ND	0.005 µg L^{-1}	USA	Nguyen et al. 2004
	disulfoton sulfoxide	disulfoton	ND	0.016 µg L^{-1}	USA	Nguyen et al. 2004
	fenamiphos sulfone	fenamiphos	0.011 µg L^{-1} [c]	0.008 µg L^{-1}	USA	Nguyen et al. 2004
	fenamiphos sulfoxide	fenamiphos	0.022 µg L^{-1} [c]	0.008 µg L^{-1}	USA	Nguyen et al. 2004
	malaoxon	malathion	0.106 µg L^{-1} [c]	0.005 µg L^{-1}	USA	Nguyen et al. 2004
	hydroxymetolachlor	metolachlor	61 ng L^{-1} [b]	1 ng L^{-1}	USA	Hladik et al. 2006
	deschlorometolachlor	metolachlor	30 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
	metolachlor morpholinone	metolachlor	37 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
	metolachlor propanol	metolachlor	73 ng L^{-1} [b]	0.2 ng L^{-1}	USA	Hladik et al. 2006
	deschloroacetylmetachlor	metolachlor	35 ng L^{-1} [b]	0.1 ng L^{-1}	USA	Hladik et al. 2006
	deschloroacetyl metachlor propanol	metolachlor	22 ng L^{-1} [b]	0.8 ng L^{-1}	USA	Hladik et al. 2006
	metachlor oxanilic acid	metolachlor	215 ng L^{-1} [b]	7 ng L^{-1}	USA	Hladik et al. 2006
	metachlor ethane sulfonic acid	metolachlor	1530 ng L^{-1} [b]	90 ng L^{-1}	USA	Hladik et al. 2006

a - pesticide identified in the reference as the source of the transformation product

b - peak concentration during study

c - median or mean concentration

d - calculated average concentration

e - combined transformation product concentration

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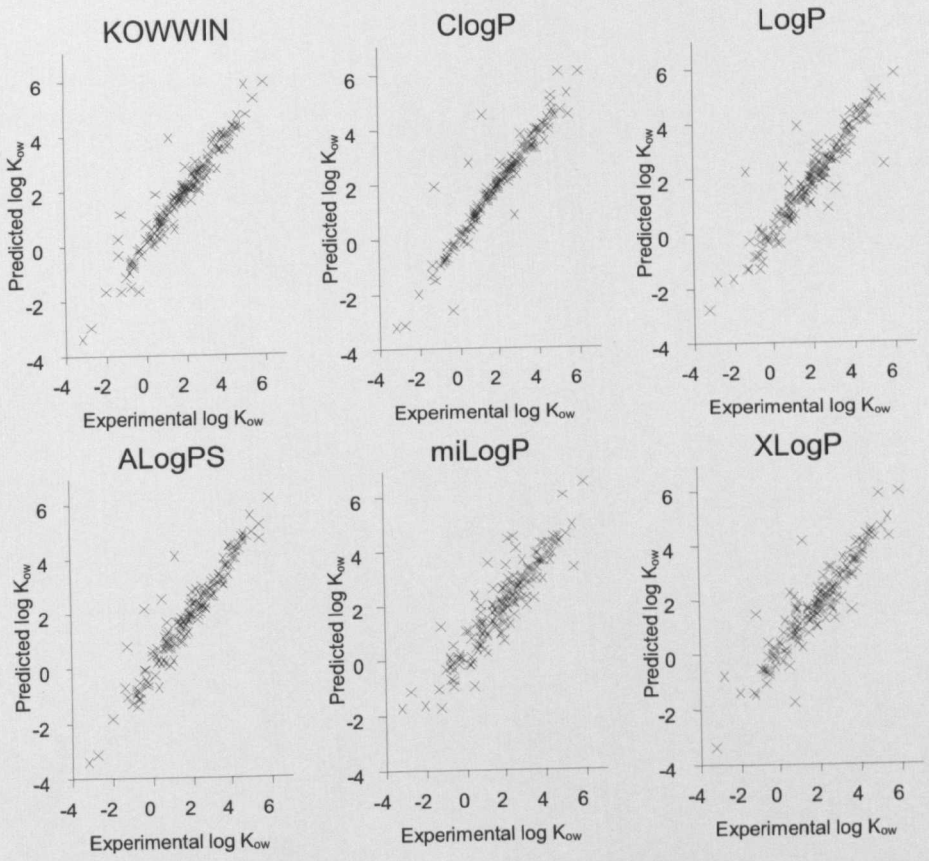

Figure B1. The predictive ability of six techniques for providing K_{ow} for transformation products (all compounds)

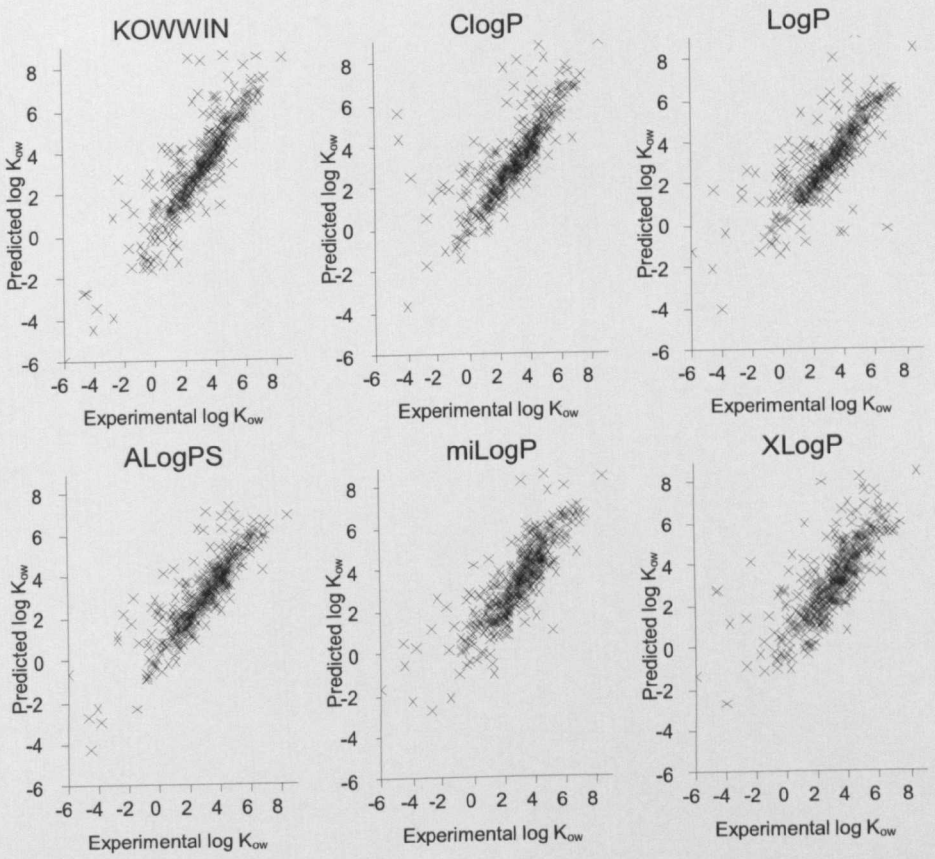

Figure B2. The predictive ability of six techniques for providing K_{ow} for pesticides (all compounds)

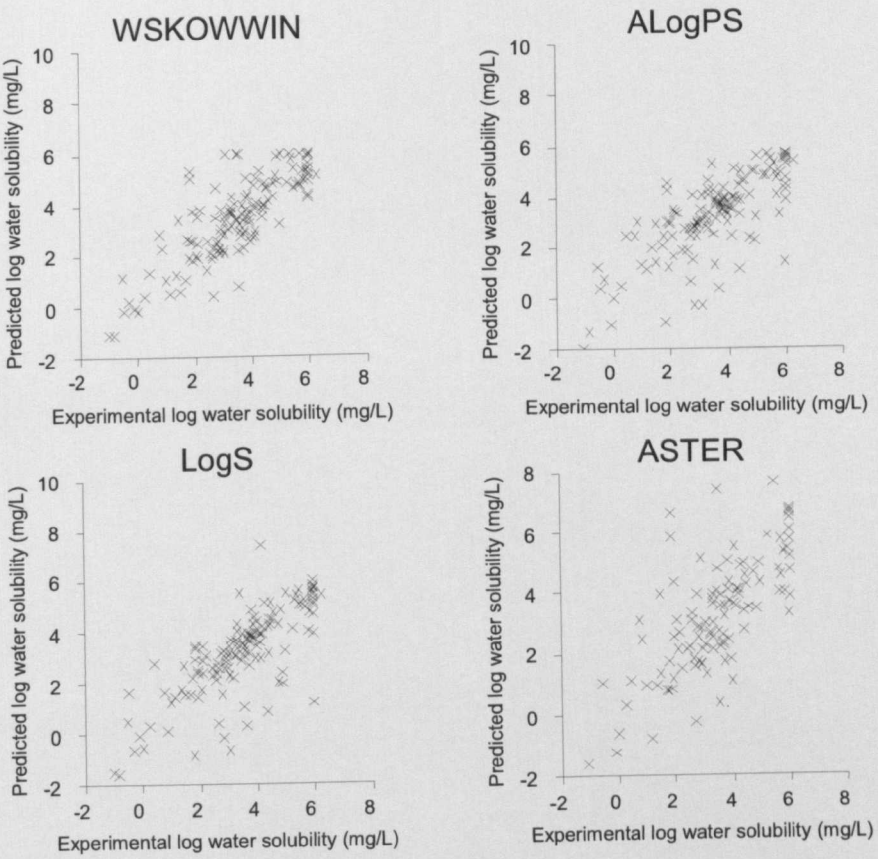

Figure B3. The predictive ability of four techniques for providing water solubility for transformation products (all compounds)

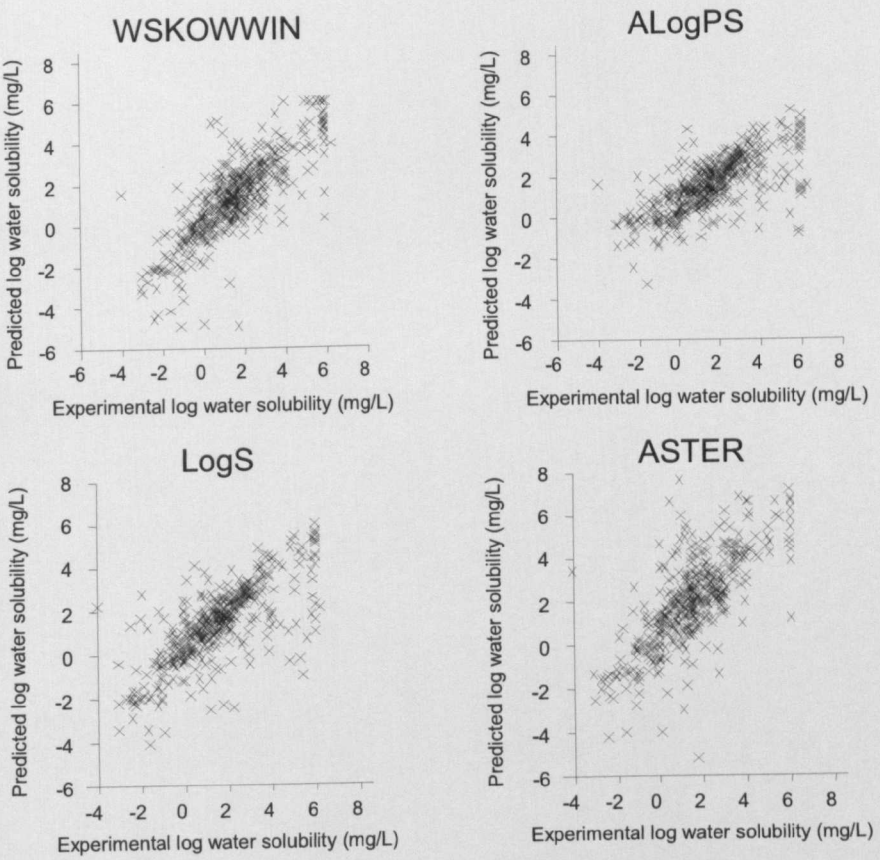

Figure B4. The predictive ability of four techniques for providing water solubility for pesticides (all compounds)

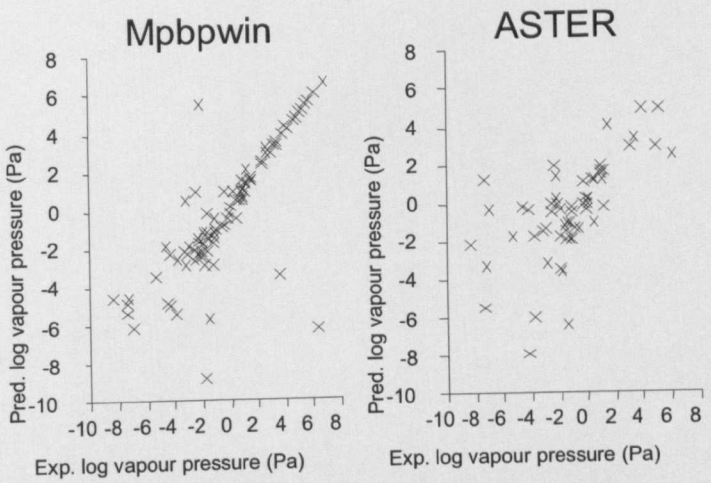

Figure B5. The predictive ability of two techniques for providing vapour pressure data for transformation products (all compounds)

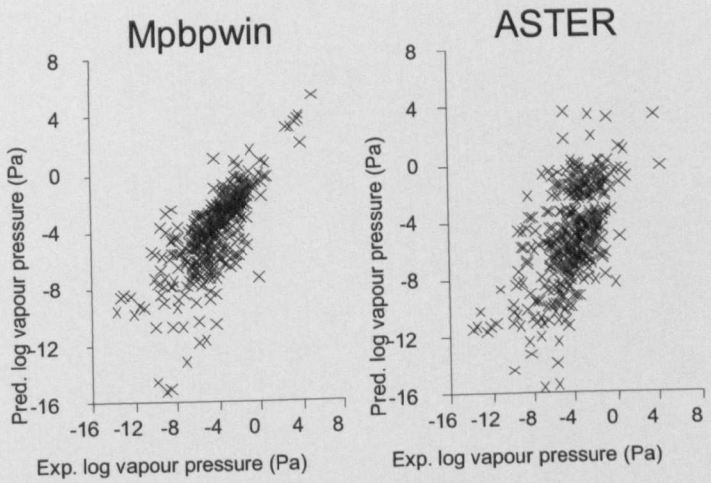

Figure B6. The predictive ability of two techniques for providing vapour pressure data for transformation products (all compounds)

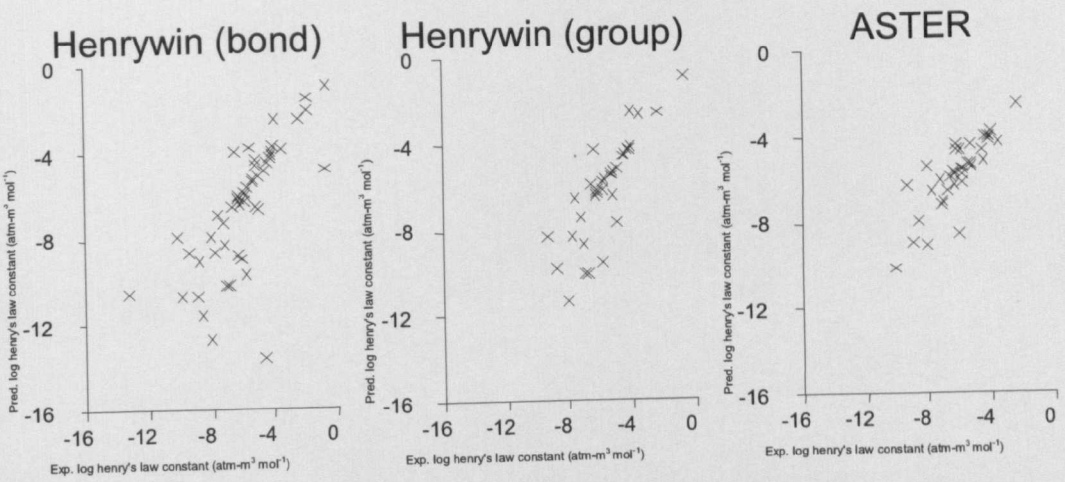

Figure B7. The predictive ability of three techniques for providing henry's law constant data for transformation products (all compounds)

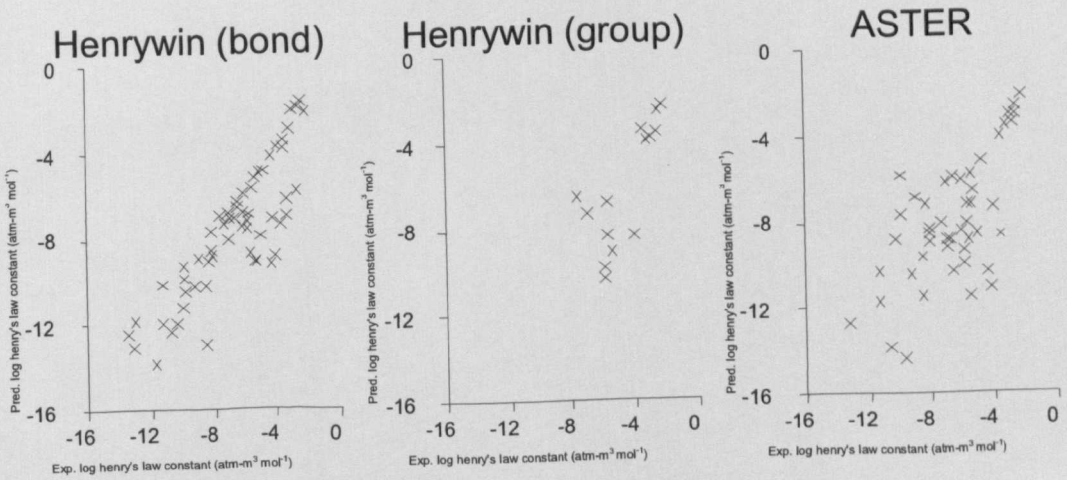

Figure B8. The predictive ability of three techniques for providing henry's law constant data for pesticides (all compounds)

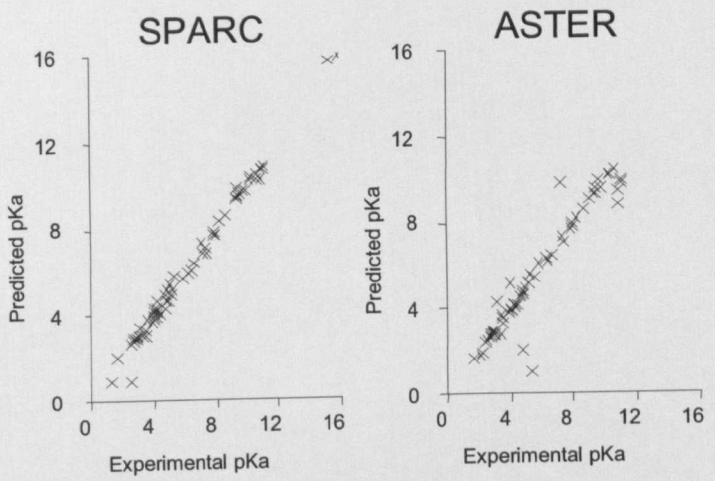

Figure B9. The predictive ability of two techniques for providing dissociation (pKa) data for transformation products (all compounds)

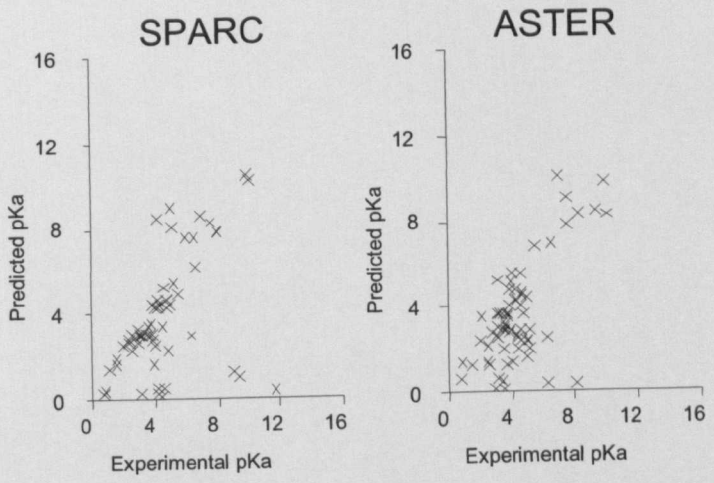

Figure B10. The predictive ability of two techniques for providing dissociation (pKa) data for pesticides (all compounds)

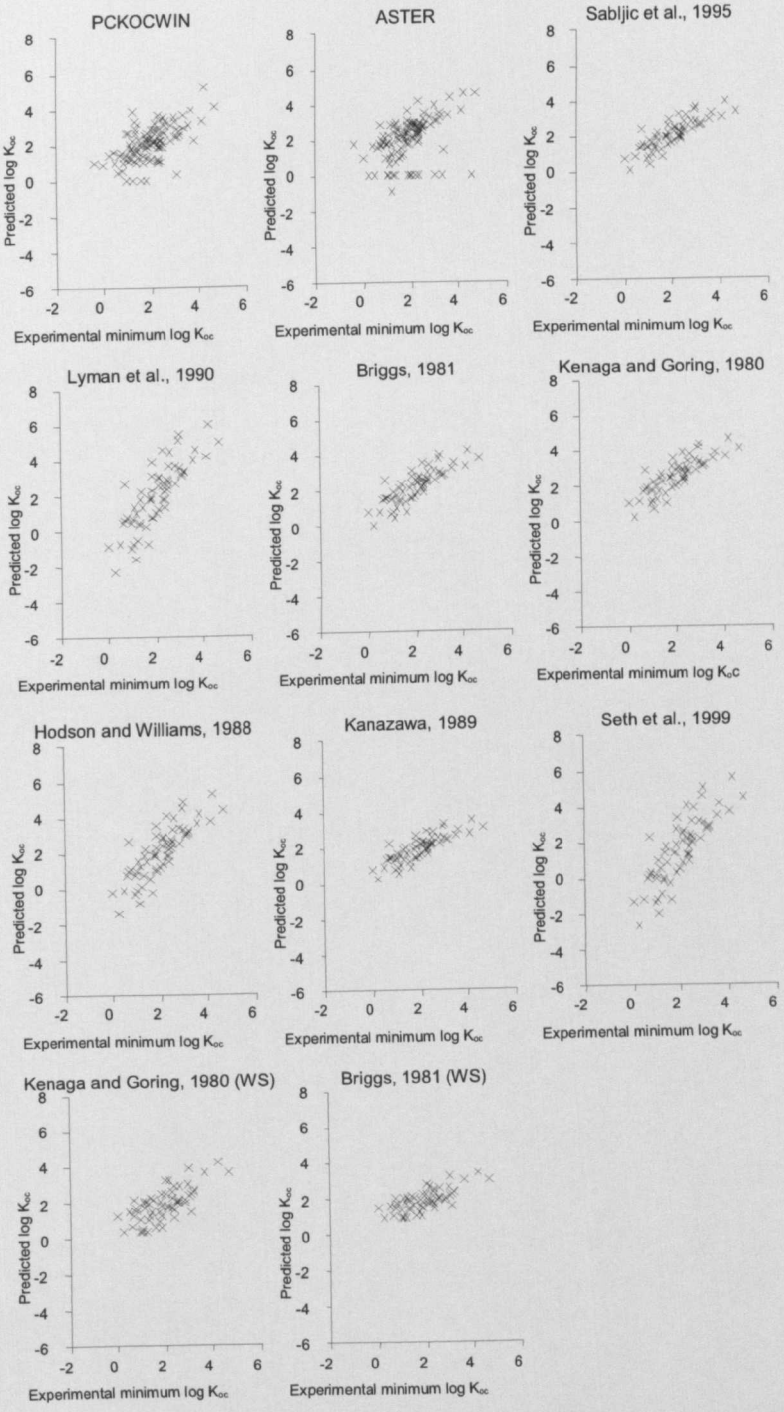

Figure B11. The predictive ability of eleven techniques for providing minimum soil sorption coefficient data for transformation products (all compounds)

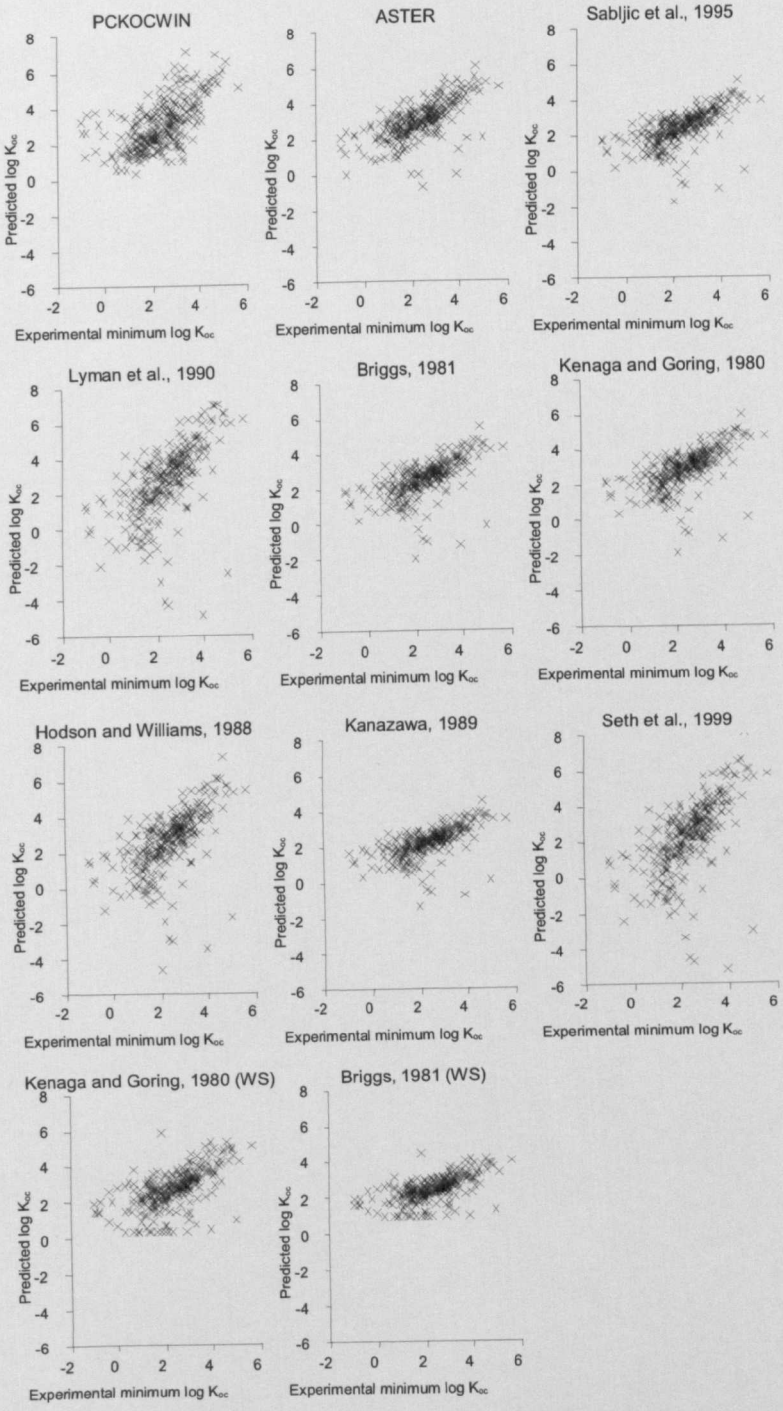

Figure B12. The predictive ability of eleven techniques for providing minimum soil sorption coefficient data for pesticides (all compounds)

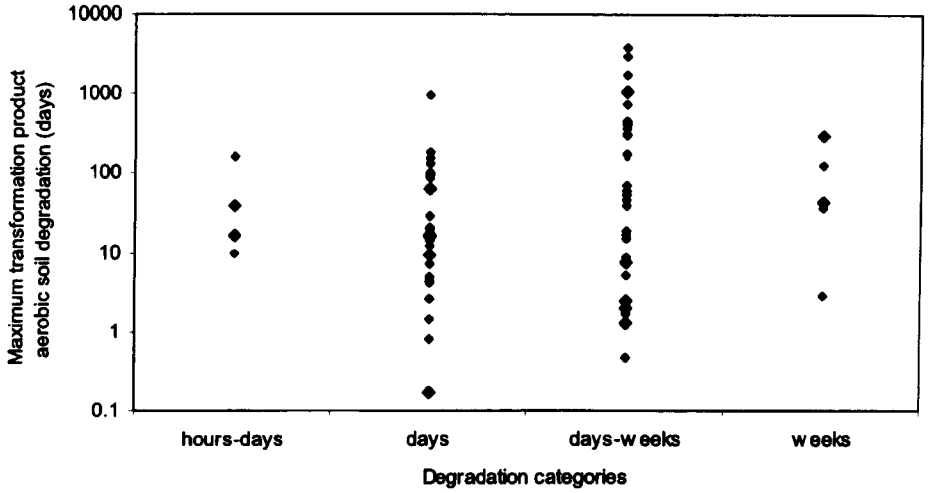

Figure B13. The predictive ability of the BIOWIN primary degradation survey model evaluated against experimental transformation product aerobic soil degradation rates

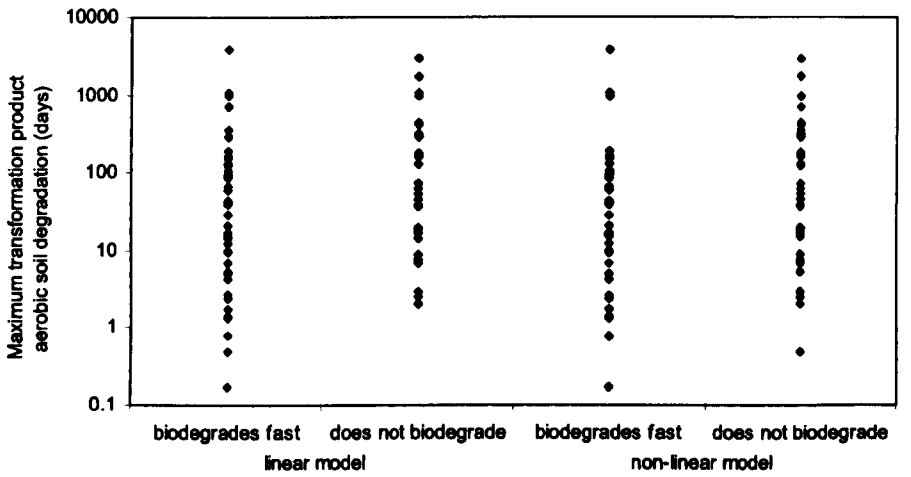

Figure B14. The predictive ability of the BIOWIN linear and non-linear models evaluated against experimental transformation product aerobic soil degradation rates

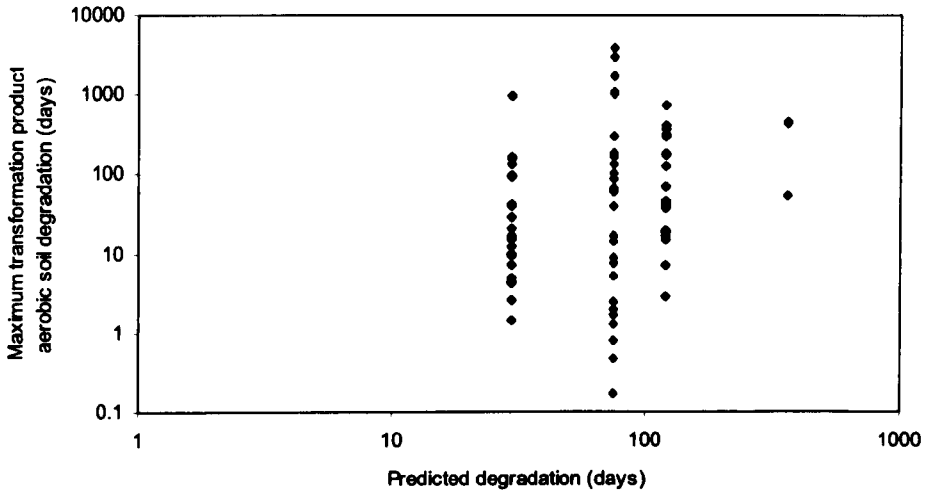

Figure B15. The predictive ability of the PBT Profiler evaluated against experimental transformation product aerobic soil degradation rates

Table B1. The summary statistics for techniques predicting K_{ow} for transformation products

Summary statistics	Optimum	KOWWIN	CLogP	LogP	ALogPS	miLogP	XLogP
All transformation products							
number of compounds[a]	160	160	157	160	159	160	159
% of positive deviations[a]	0	7.5	0.3	1.9	3.5	-5	9.1[b]
mean absolute deviation (log units)[a]	0	0.282	0.239	0.351	0.3	0.516	0.433
maximum absolute deviation (log units)	0	2.66	3.29	3.62	2.9	2.52	2.98
minimum absolute deviation (log units)	0	0	0	0	0.01	0	0
mean square absolute deviation (log units)[a]	0	0.211	0.28	0.362	0.25	0.512	0.42
% of compounds > 1 orders of magnitude[a]	0	3.13	4.46	5	3.14	13.13	7.55
% of compounds > 2 orders of magnitude	0	1.25	2.55	1.88	2.52	3.13	2.52
% of compounds > 3 orders of magnitude	0	0	1.27	0.63	0	0	0
pearson correlation coefficient[a]	1	0.965	0.954	0.938	0.958	0.916	0.927
slope	1	0.931	0.954	0.877	0.953	0.840	0.857
intercept	0	0.126	0.103	0.254	0.119	0.460	0.243
mean rank	0	0.41	0.49	0.45	0.42	0.76	0.74
Common transformation products							
number of compounds	-	156	156	156	156	156	156
% of positive deviations[a]	0	7.1	0.6	2.6	3.2	-4.5	8.3[b]
mean absolute deviation (log units)[a]	0	0.278	0.24	0.335	0.3	0.516	0.425
maximum absolute deviation (log units)	0	2.66	3.29	2.95	2.9	2.52	2.98
minimum absolute deviation (log units)	0	0	0	0	0.01	0	0
mean square absolute deviation (log units)[a]	0	0.2	0.281	0.287	0.252	0.506	0.401
% of compounds > 1 orders of magnitude[a]	0	2.56	4.49	4.49	3.21	12.8	7.05
% of compounds > 2 orders of magnitude	0	1.28	2.56	1.28	2.56	3.21	1.92
% of compounds > 3 orders of magnitude	0	0	1.28	0	0	0	0
pearson correlation coefficient[a]	1	0.996	0.953	0.951	0.958	0.917	0.931
slope	1	0.94	0.954	0.899	0.956	0.848	0.863
intercept	0	0.1	0.105	0.191	0.119	0.441	0.245
mean rank	0	0.48	0.4	0.49	0.44	0.91	0.8

[a] - mean rank derived from these statistics
[b] - positive deviation from 50% identified as significant (95% confidence limits)

Table B2. The summary statistics for techniques predicting K_{ow} for pesticides

Summary statistics	Optimum	KOWWIN	CLogP	LogP	ALogPS	miLogP	XLogP
All pesticides							
number of compounds[a]	445	444	438	445	444	445	444
% of positive deviations[a]	0	-7	-11[b]	2.1	1.1	-16.3[b]	-3.4
mean absolute deviation (log units)[a]	0	0.62	0.647	0.686	0.603	0.81	0.834
maximum absolute deviation (log units)	0	6.2	10.19	6.98	5.34	6.87	7.31
minimum absolute deviation (log units)	0	0	0	0	0	0	0
mean square absolute deviation (log units)[a]	0	1.082	1.511	1.443	0.962	1.42	1.632
% of compounds > 1 orders of magnitude[a]	0	17.79	16.44	18.65	16.89	24.72	27.02
% of compounds > 2 orders of magnitude	0	6.98	7.31	8.76	5.63	7.19	7.43
% of compounds > 3 orders of magnitude	0	2.48	4.11	4.27	2.93	3.37	3.6
pearson correlation coefficient[a]	1	0.879	0.806	0.8	0.8716	0.837	0.783
slope	1	0.935	0.777	0.685	0.762	0.792	0.72
intercept	0	0.449	1.009	1.1	0.878	1.073	1.062
mean rank	0	0.53	0.81	0.57	0.46	0.75	0.73
Common pesticides							
number of compounds	-	437	437	437	437	437	437
% of positive deviations[a]	0	-7.2	-10.9[b]	2.9	1.3	-16.6[b]	-3.3
mean absolute deviation (log units)[a]	0	0.626	0.644	0.667	0.596	0.805	0.818
maximum absolute deviation (log units)	0	6.2	10.19	6.98	4.55	6.87	7.31
minimum absolute deviation (log units)	0	0	0	0	0	0	0
mean square absolute deviation (log units)[a]	0	1.098	1.508	1.356	0.9088	1.392	1.547
% of compounds > 1 orders of magnitude[a]	0	18.07	16.25	18.07	16.7	24.71	26.77
% of compounds > 2 orders of magnitude	0	7.09	7.32	8.24	5.49	7.09	7.09
% of compounds > 3 orders of magnitude	0	2.52	4.12	3.89	2.75	3.2	3.2
pearson correlation coefficient[a]	1	0.872	0.806	0.803	0.873	0.834	0.7858
slope	1	0.929	0.779	0.698	0.775	0.798	0.735
intercept	0	0.476	1.004	1.050	0.837	1.059	1.011
mean rank	0	0.64	0.79	0.69	0.52	0.92	0.84

[a] - mean rank derived from these statistics
[b] - positive deviation from 50% identified as significant (95% confidence limits)

Table B3. The summary statistics for all combinations of the four most accurate methods for providing transformation product K_{ow} predictions

Summary statistics	Optimum	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
Common transformation products																
number of compounds	-	156	156	156	156	156	156	156	156	156	156	156	156	156	156	156
% of positive deviations[a]	0	7.1	0.6	2.6	3.2	3.8	7.1	7.1	3.2	4.5	1.3	4.5	3.8	5.1	1.3	3.8
mean absolute deviation (log units)[a]	0	0.278	0.24	0.335	0.3	0.229	0.26	0.244	0.251	0.229	0.284	0.229	0.215	0.244	0.233	0.221
maximum absolute deviation (log units)	0	2.66	3.29	2.95	2.9	2.98	2.69	2.78	3.01	3.1	2.81	2.89	2.95	2.76	2.97	2.89
minimum absolute deviation (log units)	0	0	0	0	0	0	0	0	<0.01	0	<0.01	<0.01	<0.01	0	0	<0.01
mean square absolute deviation (log units)[a]	0	0.2	0.281	0.287	0.252	0.205	0.174	0.169	0.217	0.195	0.217	0.179	0.172	0.167	0.188	0.167
% of compounds > 1 orders of magnitude[a]	0	2.56	4.49	4.49	3.21	2.56	3.21	1.92	3.85	2.56	4.49	3.85	1.92	2.56	3.21	3.21
% of compounds > 2 orders of magnitude	0	1.28	2.56	1.28	2.56	1.28	0.64	1.28	1.92	1.92	0.64	1.28	1.28	0.64	1.92	1.28
% of compounds > 3 orders of magnitude	0	0	1.28	0	0	0	0	0	0.64	0.64	0	0	0	0	0	0
pearson correlation coefficient[a]	1	0.966	0.953	0.951	0.958	0.965	0.971	0.972	0.963	0.967	0.963	0.97	0.971	0.972	0.968	0.972
slope	1	0.94	0.954	0.899	0.956	0.947	0.92	0.948	0.926	0.955	0.927	0.931	0.95	0.932	0.936	0.937
intercept	0	0.1	0.105	0.191	0.119	0.103	0.146	0.109	0.148	0.112	0.155	0.132	0.108	0.137	0.138	0.129
mean rank	0	0.76	0.75	0.87	0.76	0.64	0.74	0.67	0.71	0.65	0.71	0.68	0.56	0.64	0.58	0.61

[a] - mean rank derived from these statistics

Key to the combinations of predictive techniques examined:

A - KOWWIN
B - CLogP
C - LogP
D - ALogPS
E - KOWWIN & CLogP
F - KOWWIN & LogP
G - KOWWIN & ALogPS
H - CLogP & LogP
I - CLogP & ALogPS
J - LogP & ALogPS
K - KOWWIN, CLogP & LogP
L - KOWWIN, CLogP & ALogPS
M - KOWWIN, LogP & ALogPS
N - CLogP, LogP & ALogPS
O - KOWWIN, CLogP, LogP & ALogPS

Table B4. The summary statistics for techniques predicting water solubility (mg L^{-1}) for transformation products

Summary statistics	Optimum	WSKOWWIN	ALogPS	LogS	ASTER
All transformation products					
number of compounds[a]	139	139	137	137	113
% of positive deviations[a]	0	11.9	6.2	7.7	11.9
mean absolute deviation (log units)[a]	0	0.719	0.828	0.765	1.011
maximum absolute deviation (log units)	0	3.44	4.51	4.76	4.74
minimum absolute deviation (log units)	0	0	0	0	0.02
mean square absolute deviation (log units)[a]	0	0.975	1.408	1.363	1.898
% of compounds > 1 orders of magnitude[a]	0	21.58	27.74	24.09	38.94
% of compounds > 2 orders of magnitude	0	5.76	10.95	11.68	14.16
% of compounds > 3 orders of magnitude	0	1.44	3.65	3.65	4.42
pearson correlation coefficient[a]	1	0.829	0.755	0.78	0.722
slope	1	0.814	0.712	0.786	0.873
intercept	0	0.632	0.779	0.480	0.296
mean rank	0	0.59	0.65	0.62	1
Common transformation products					
number of compounds	-	113	113	113	113
% of positive deviations[a]	0	12.8	5.8	8.4	11.9
mean absolute deviation (log units)[a]	0	0.724	0.889	0.796	1.011
maximum absolute deviation (log units)	0	3.44	4.51	4.76	4.74
minimum absolute deviation (log units)	0	0	0	0	0.02
mean square absolute deviation (log units)[a]	0	0.973	1.617	1.474	1.898
% of compounds > 1 orders of magnitude[a]	0	21.24	30.97	25.66	38.94
% of compounds > 2 orders of magnitude	0	5.31	13.27	12.39	14.16
% of compounds > 3 orders of magnitude	0	1.77	4.42	4.42	4.42
pearson correlation coefficient[a]	1	0.81	0.693	0.744	0.722
slope	1	0.783	0.664	0.759	0.873
intercept	0	0.667	0.885	0.512	0.296
mean rank	0	0.68	0.8	0.75	0.97

[a] - mean rank derived from these statistics

Table B5. The summary statistics for techniques predicting water solubility (mg L^{-1}) for pesticides

Summary statistics	Optimum	WSKOWWIN	ALogPS	LogS	ASTER
All pesticides					
number of compounds[a]	463	463	460	460	424
% of positive deviations[a]	0	8.5[b]	-6.5	-0.2	-19.6[b]
mean absolute deviation (log units)[a]	0	0.855	0.975	0.848	1.106
maximum absolute deviation (log units)	0	11.47	6.64	6.41	7.43
minimum absolute deviation (log units)	0	0	0	<0.01	<0.01
mean square absolute deviation (log units)[a]	0	7.76	2.036	1.831	2.452
% of compounds > 1 orders of magnitude[a]	0	31.32	34.35	25.22	39.62
% of compounds > 2 orders of magnitude	0	6.91	12.83	11.96	13.68
% of compounds > 3 orders of magnitude	0	3.24	5.22	5.65	6.37
pearson correlation coefficient[a]	1	0.793	0.683	0.736	0.74
slope	1	0.842	0.455	0.639	0.863
intercept	0	0.003	0.887	0.426	0.749
mean rank	0	0.57	0.68	0.52	0.97
Common pesticides					
number of compounds	-	423	423	423	423
% of positive deviations[a]	0	8.9[b]	-8.2	-3.2	-19.5[b]
mean absolute deviation (log units)[a]	0	0.793	0.879	0.762	1.108
maximum absolute deviation (log units)	0	6.6	5.7	6.18	7.43
minimum absolute deviation (log units)	0	0	0	<0.01	<0.01
mean square absolute deviation (log units)[a]	0	1.359	1.547	1.388	2.457
% of compounds > 1 orders of magnitude[a]	0	29.31	31.44	23.4	39.72
% of compounds > 2 orders of magnitude	0	5.44	10.64	9.69	13.71
% of compounds > 3 orders of magnitude	0	2.6	3.31	3.55	6.38
pearson correlation coefficient[a]	1	0.807	0.743	0.778	0.74
slope	1	0.806	0.521	0.703	0.863
intercept	0	0.045	0.846	0.408	0.75
mean rank	0	0.64	0.72	0.57	1

[a] - mean rank derived from these statistics
[b] - positive deviation from 50% identified as significant (95% confidence limits)

Table B6. The summary statistics for techniques predicting vapour pressure (Pa) and henry's law constant (atm-m^3 mol^{-1}) for transformation products

Summary statistics	Optimum	Mpbpwin	ASTER	Optimum	Henrywin-bond	Henrywin-group	ASTER
All transformation products							
number of compounds[a]	93	93	59	50	50	34	36
% of positive deviations[a]	0	0.5	-17.8[b]	0	6	8.8	-22.2
mean absolute deviation (log units)[a]	0	1.716	1.766	0	1.241	0.866	0.677
maximum absolute deviation (log units)	0	29.02	8.59	0	9.09	3.73	3.17
minimum absolute deviation (log units)	0	0	0.04	0	<0.01	<0.01	<0.01
mean square absolute deviation (log units)[a]	0	21.612	6.41	0	4.369	2	1.104
% of compounds > 1 orders of magnitude[a]	0	26.88	50.85	0	36	32.35	22.22
% of compounds > 2 orders of magnitude	0	16.13	32.2	0	24	17.65	8.33
% of compounds > 3 orders of magnitude	0	11.83	20.34	0	12	11.76	2.78
pearson correlation coefficient[a]	1	0.362	0.638	1	0.727	0.825	0.826
slope	1	0.485	0.535	1	0.885	1.133	0.796
intercept	0	-0.671	0.271	0	-1.310	0.386	-0.873
mean rank	0	0.59	0.81	0	0.71	0.73	0.73
Common transformation products							
number of compounds	-	59	59	-	27	27	27
% of positive deviations[a]	0	-0.8	-17.8[b]	0	-1.9	5.6	-24.1
mean absolute deviation (log units)[a]	0	2.09	1.766	0	0.663	0.816	0.727
maximum absolute deviation (log units)	0	29.02	8.59	0	3.84	3.73	3.17
minimum absolute deviation (log units)	0	0	0.04	0	<0.01	<0.01	<0.01
mean square absolute deviation (log units)[a]	0	29.363	6.41	0	1.569	1.991	1.18
% of compounds > 1 orders of magnitude[a]	0	35.59	50.85	0	18.52	29.63	25.93
% of compounds > 2 orders of magnitude	0	18.64	32.2	0	11.11	14.81	7.41
% of compounds > 3 orders of magnitude	0	11.86	20.34	0	11.11	14.81	3.7
pearson correlation coefficient[a]	1	0.029	0.638	1	0.822	0.833	0.799
slope	1	0.044	0.535	1	1.105	1.27	0.56
intercept	0	-1.916	0.271	0	0.145	1.113	-1.956
mean rank	0	0.75	0.69	0	0.64	0.81	0.89

[a] - mean rank derived from these statistics
[b] - positive deviation from 50% identified as significant (95% confidence limits)

Table B7. The summary statistics for techniques predicting vapour pressure (Pa) and henry's law constant (atm-m^3 mol^{-1}) for pesticides

Summary statistics	Optimum	Mpbpwin	ASTER	Optimum	Henrywin-bond	Henrywin-group	ASTER
All pesticides							
number of compounds[a]	410	408	390	61	60	14	47
% of positive deviations[a]	0	-11.8[b]	11[b]	0	11.7	35.7	26.6[b]
mean absolute deviation (log units)[a]	0	1.439	2.343	0	1.461	1.699	1.972
maximum absolute deviation (log units)	0	11.05	9.69	0	12.96	4.46	6.91
minimum absolute deviation (log units)	0	<0.01	0.04	0	<0.01	0.04	<0.01
mean square absolute deviation (log units)[a]	0	4.06	8.224	0	6.069	5.514	6.97
% of compounds > 1 orders of magnitude[a]	0	52.7	77.95	0	46.67	50	61.7
% of compounds > 2 orders of magnitude	0	24.02	50.26	0	23.33	35.71	42.55
% of compounds > 3 orders of magnitude	0	11.03	29.74	0	16.67	28.57	27.66
pearson correlation coefficient[a]	1	0.736	0.582	1	0.756	0.769	0.668
slope	1	0.781	0.784	1	0.83	1.212	0.725
intercept	0	-0.637	-1.665	0	-2.241	-0.556	-3.19
mean rank	0	0.59	0.99	0	0.58	0.86	0.84
Common pesticides							
number of compounds	-	388	388	-	12	12	12
% of positive deviations[a]	0	-13.1[b]	10.8[b]	0	0	41.7	33.3
mean absolute deviation (log units)[a]	0	1.391	2.344	0	1.24	1.545	1.289
maximum absolute deviation (log units)	0	11.05	9.69	0	3.66	4.46	4.03
minimum absolute deviation (log units)	0	<0.01	0.04	0	0.06	0.04	<0.01
mean square absolute deviation (log units)[a]	0	3.691	8.235	0	2.637	4.885	3.422
% of compounds > 1 orders of magnitude[a]	0	52.32	78.09	0	58.33	41.67	41.67
% of compounds > 2 orders of magnitude	0	22.94	50.26	0	16.67	33.33	25
% of compounds > 3 orders of magnitude	0	9.79	29.64	0	16.67	25	16.67
pearson correlation coefficient[a]	1	0.716	0.582	1	0.943	0.891	0.882
slope	1	0.726	0.784	1	1.668	1.568	1.442
intercept	0	-0.815	-1.657	0	2.182	0.95	0.772
mean rank	0	0.68	0.96	0	0.57	0.93	0.84

[a] - mean rank derived from these statistics
[b] - positive deviation from 50% identified as significant (95% confidence limits)

Table B8. The summary statistics for techniques predicting dissociation (pKa) for transformation products

Summary statistics	Optimum	SPARC	ASTER
All transformation products			
number of compounds[a]	90	66	68
% of positive deviations[a]	0	3	13.2
mean absolute deviation[a]	0	0.245	0.35
maximum absolute deviation	0	1.67	4.39
minimum absolute deviation	0	<0.01	0
mean square absolute deviation[a]	0	0.117	0.693
% of compounds > 1 pH unit[a]	0	1.52	11.76
% of compounds > 2 pH units	0	0	4.41
% of compounds > 3 pH units	0	0	1.47
pearson correlation coefficient[a]	1	0.994	0.954
slope	1	0.998	0.952
intercept	0	-0.025	0.138
mean rank	0	0.39	0.99
Common transformation products			
number of compounds	-	50	50
% of positive deviations[a]	0	6	8
mean absolute deviation[a]	0	0.203	0.327
maximum absolute deviation	0	0.7	2.77
minimum absolute deviation	0	0.012	0
mean square absolute deviation[a]	0	0.063	0.517
% of compounds > 1 pH unit[a]	0	0	12
% of compounds > 2 pH units	0	0	4
% of compounds > 3 pH units	0	0	0
pearson correlation coefficient[a]	1	0.996	0.966
slope	1	0.975	0.939
intercept	0	0.116	0.301
mean rank	0	0.32	1

[a] - mean rank derived from these statistics

Table B9. The summary statistics for techniques predicting dissociation (pKa) for pesticides

Summary statistics	Optimum	SPARC	ASTER
All pesticides			
number of compounds[a]	163	63	72
% of positive deviations[a]	0	7.1	15.3
mean absolute deviation[a]	0	1.389	1.293
maximum absolute deviation	0	11.28	7.75
minimum absolute deviation	0	<0.01	0
mean square absolute deviation[a]	0	6.489	3.589
% of compounds > 1 pH unit[a]	0	30.16	45.83
% of compounds > 2 pH units	0	22.22	25
% of compounds > 3 pH units	0	17.46	9.72
pearson correlation coefficient[a]	1	0.493	0.679
slope	1	0.565	0.836
intercept	0	1.301	-0.034
mean rank	0	0.85	0.84
Common pesticides			
number of compounds	-	38	38
% of positive deviations[a]	0	5.3	10.5
mean absolute deviation[a]	0	0.597	0.838
maximum absolute deviation	0	3.31	3.76
minimum absolute deviation	0	<0.01	0
mean square absolute deviation[a]	0	0.891	1.589
% of compounds > 1 pH unit[a]	0	15.79	31.58
% of compounds > 2 pH units	0	7.89	13.16
% of compounds > 3 pH units	0	2.63	5.26
pearson correlation coefficient[a]	1	0.915	0.853
slope	1	1.071	1.035
intercept	0	-0.477	-0.399
mean rank	0	0.57	1

[a] - mean rank derived from these statistics

Table B10. The summary statistics for techniques predicting minimum soil sorption coefficient for transformation products

Summary statistics	Optimum	PCKOCWIN	ASTER	Sabljic et al. 1995	Lyman et al. 1990	Briggs 1981	Kenaga and Goring 1980	Hodson and Williams 1988	Kanazawa 1989	Seth et al. 1999	Kenaga and Goring 1980	Briggs 1981
All transformation products												
number of compounds[a]	-	110	110	64	64	64	64	64	64	64	61	61
% of positive deviations[a]	0	-10	-16.4[b]	-3.1	-6.3	-9.4	-39.1[b]	-1.6	1.6	21.9[b]	7.4	7.4
mean absolute deviation (log units)[a]	0	0.674	0.823	0.459	0.831	0.478	0.588	0.628	0.462	0.925	0.609	0.571
maximum absolute deviation (log units)	0	2.78	4.56	1.71	5.7	1.88	2.21	1.95	1.58	3.13	1.63	1.63
minimum absolute deviation (log units)	0	0.01	0.01	0.01	0	0.01	0	0.01	0.01	0.01	0	0.01
mean square absolute deviation (log units)[a]	0	0.733	1.264	0.308	1.257	0.356	0.59	0.697	0.322	1.456	0.512	0.463
% of compounds > 1 orders of magnitude[a]	0	20	29.09	6.25	31.25	4.69	23.44	21.88	4.69	39.06	13.11	8.20
% of compounds > 2 orders of magnitude	0	1.82	8.18	0	10.94	0	1.56	0	0	10.94	0	0
% of compounds > 3 orders of magnitude	0	0	1.82	0	0	0	0	0	0	1.56	0	0
pearson correlation coefficient[a]	1	0.585	0.44	0.826	0.826	0.826	0.826	0.826	0.826	0.826	0.701	0.701
slope	1	0.623	0.556	0.689	1.509	0.763	0.798	1.213	0.59	1.51	0.667	0.432
intercept	0	0.865	1.03	0.699	-1.037	0.687	0.924	-0.395	0.736	-1.467	0.559	1.015
mean rank	0	0.55	0.78	0.25	0.61	0.29	0.59	0.41	0.24	0.77	0.41	0.37
Common transformation products												
number of compounds[a]	-	55	55	55	55	55	55	55	55	55	55	55
% of positive deviations[a]	0	-13.6	-19.1	-2.7	-0.9	-8.2	-42.7[b]	0.9	0.9	19.1	8.2	8.2
mean absolute deviation (log units)[a]	0	0.676	0.704	0.455	0.863	0.473	0.583	0.644	0.455	0.966	0.594	0.572
maximum absolute deviation (log units)	0	1.96	3	1.71	2.7	1.88	2.21	1.95	1.58	3.13	1.63	1.63
minimum absolute deviation (log units)	0	0.01	0.01	0.02	<0.01	0.03	<0.01	0.04	0.01	0.01	<0.01	0.01
mean square absolute deviation (log units)[a]	0	0.646	0.927	0.296	1.278	0.35	0.596	0.694	0.302	1.493	0.492	0.473
% of compounds > 1 orders of magnitude[a]	0	18.18	23.64	3.64	32.73	3.64	25.42	21.82	3.64	41.82	10.91	9.09
% of compounds > 2 orders of magnitude	0	0	5.45	0	10.91	0	1.82	0	0	10.91	0	0
% of compounds > 3 orders of magnitude	0	0	0	0	0	0	0	0	0	1.82	0	0
pearson correlation coefficient[a]	1	0.717	0.669	0.839	0.839	0.839	0.839	0.839	0.839	0.839	0.732	0.732
slope	1	0.775	0.825	0.71	1.554	0.785	0.821	1.249	0.607	1.555	0.677	0.438
intercept	0	0.662	0.636	0.666	-1.108	0.651	0.886	-0.453	0.708	-1.539	0.537	1.002
mean rank	0	0.55	0.67	0.26	0.61	0.3	0.62	0.43	0.25	0.79	0.44	0.43

[a] - mean rank derived from these statistics
[b] - positive deviation from 50% identified as significant (95% confidence limits)

Table B11. The summary statistics for techniques predicting minimum soil sorption coefficient for pesticides

Summary statistics	Optimum	PCKOCWIN	ASTER	Sabljic et al. 1995	Lyman et al. 1990	Briggs 1981	Kenaga and Goring 1980	Hodson and Williams 1988	Kanazawa 1989	Seth et al. 1999	Kenaga and Goring 1980	Briggs 1981
All pesticides												
number of compounds[a]	-	299	279	290	290	290	290	290	290	290	298	298
% of positive deviations[a]	0	-24.6[b]	-33.9[b]	-4.5	-18.3[b]	-16.9[b]	-29[b]	-16.2[b]	11[b]	-3.1	-19.8[b]	0.3
mean absolute deviation (log units)[a]	0	0.976	0.881	0.628	1.192	0.68	0.844	0.93	0.645	1.094	0.733	0.655
maximum absolute deviation (log units)	0	6.9	3.92	5.01	8.73	5.14	5	7.35	4.87	9.17	4.05	3.73
minimum absolute deviation (log units)	0	0	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
mean square absolute deviation (log units)[a]	0	1.785	1.271	0.891	2.842	0.994	1.263	1.839	0.866	2.771	1.063	0.814
% of compounds > 1 orders of magnitude[a]	0	34.45	34.05	18.62	45.86	19.31	28.62	32.41	18.62	39.31	28.19	19.8
% of compounds > 2 orders of magnitude	0	11.71	7.89	4.48	15.86	4.83	6.9	7.93	4.83	15.52	6.38	5.37
% of compounds > 3 orders of magnitude	0	3.68	1.43	1.72	4.83	1.72	2.41	2.76	1.38	4.48	1.34	0.34
pearson correlation coefficient[a]	1	0.584	0.644	0.59	0.59	0.59	0.59	0.59	0.59	0.59	0.604	0.604
slope	1	0.715	0.591	0.494	1.083	0.547	0.572	0.87	0.423	1.084	0.557	0.36
intercept	0	1.321	1.594	1.222	0.109	1.266	1.53	0.525	1.184	-0.321	1.395	1.557
mean rank	0	0.78	0.76	0.47	0.91	0.57	0.72	0.72	0.51	0.77	0.63	0.45
Common pesticides												
number of compounds[a]	-	274	274	274	274	274	274	274	274	274	274	274
% of positive deviations[a]	0	-26.3[b]	-33.6[b]	-6.2	-20.4[b]	-18.6[b]	-30.3[b]	-18.2[b]	10.2[b]	-4.4	-21.2[b]	-0.7
mean absolute deviation (log units)[a]	0	0.909	0.875	0.623	1.164	0.678	0.85	0.909	0.641	1.051	0.7	0.631
maximum absolute deviation (log units)	0	4.14	3.92	5.01	8.73	5.14	5	7.35	4.87	9.17	4.05	3.73
minimum absolute deviation (log units)	0	0.02	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
mean square absolute deviation (log units)[a]	0	1.465	1.249	0.888	2.785	0.997	1.288	1.804	0.858	2.657	0.984	0.762
% of compounds > 1 orders of magnitude[a]	0	32.12	33.94	18.25	44.16	18.98	28.47	31.39	18.25	37.23	25.91	18.61
% of compounds > 2 orders of magnitude	0	9.49	7.66	4.38	14.6	4.74	7.3	7.66	4.74	13.87	5.47	4.74
% of compounds > 3 orders of magnitude	0	2.55	1.09	1.82	4.38	1.82	2.55	2.55	1.46	4.01	1.46	0.36
pearson correlation coefficient[a]	1	0.651	0.641	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.643	0.643
slope	1	0.741	0.595	0.491	1.074	0.543	0.568	0.864	0.42	1.076	0.582	0.377
intercept	0	1.257	1.577	1.261	0.194	1.309	1.575	0.594	1.217	-0.236	1.362	1.535
mean rank	0	0.74	0.77	0.49	0.92	0.58	0.75	0.74	0.52	0.77	0.61	0.43

[a] - mean rank derived from these statistics
[b] - positive deviation from 50% identified as significant (95% confidence limits)

Table B12. The summary statistics for all combinations of the most accurate methods for providing minimum transformation product K_{oc} predictions

Summary statistics	Optimum	A	B	C	D	E	F	G
Common transformation products								
number of compounds[a]	-	53	53	53	53	53	53	53
% of positive deviations[a]	0	-2.8	-8.5	0.9	-2.8	2.8	-2.8	-2.8
mean absolute deviation (log units)[a]	0	0.417	0.438	0.414	0.425	0.413	0.415	0.416
maximum absolute deviation (log units)	0	0.96	1.22	0.81	1.09	0.80	0.93	0.94
minimum absolute deviation (log units)	0	0.02	0.03	0.01	0	0	0.01	0.02
mean square absolute deviation (log units)[a]	0	0.224	0.279	0.223	0.246	0.214	0.221	0.222
% of compounds > 1 orders of magnitude[a]	0	0	1.89	0	1.89	0	0	0
% of compounds > 2 orders of magnitude	0	0	0	0	0	0	0	0
% of compounds > 3 orders of magnitude	0	0	0	0	0	0	0	0
pearson correlation coefficient[a]	1	0.862	0.862	0.862	0.862	0.862	0.862	0.862
slope	1	0.777	0.860	0.665	0.819	0.721	0.763	0.767
intercept	0	0.523	0.493	0.586	0.508	0.555	0.539	0.534
mean rank	0	0.62	1	0.57	0.84	0.61	0.61	0.62

[a] - mean rank derived from these statistics

Key to the combinations of predictive techniques used:

A - Sabljić et al. 1995
B - Briggs et al. 1981
C - Kanazawa 1989
D - Sabljić et al. 1995 & Briggs et al. 1981
E - Sabljić et al. 1995 & Kanazawa 1989
F - Briggs et al. 1981 & Kanazawa 1989
G - Sabljić et al. 1995, Briggs et al. 1981 & Kanazawa 1989

Table C1. Ecotoxicity and physico-chemical property data for parent compounds and associated transformation products

Pesticide	Transformation product	log K_{ow}	pKa	Fish 96h LC_{50} (mg/L)				Daphnid 48h EC_{50} (mg/L)				Algae 72-96h EC/IC_{50} (mg/L)			
				Median	Max	Min	n	Median	Max	Min	n	Median	Max	Min	n
2,3,6-TBA		4.34	1.5	0.009	-	-	1	-	-	-	-	-	-	-	-
	2,4,5-trichlorophenol	3.72	7.4	0.902	3.06	0.0012	11	-	-	-	-	-	-	-	-
2,4-D		2.81	2.73	27.7	2779	1.4	28	25	135	1.3	9	41.77	-	-	1
	2,4-dichlorophenol	3.06	7.89	6.7	11.6	2	11	2.6	5.1	0.0026	7	11.6	14	9.2	4
	4-chlorocatechol		8.67	1.58	-	-	1	-	-	-	-	-	-	-	-
	4-chlorophenol	2.39	9.41	5.3	9	1.91	16	4.82	8.9	2.5	9	-	-	-	-
	succinic acid	-0.59	4.21	-	-	-	-	374.2	-	-	1	-	-	-	-
acephate		-0.85	none	180	2050	1.34	13	49.35	71.78	1.3	4	-	-	-	-
	methamidophos	-0.66	none	45.5	100	1.28	10	0.039	0.27	0.026	4	-	-	-	-
aldicarb		1.13	11.7	0.861	10.06	0.05	15	0.497	0.74	0.075	4	-	-	-	-
	aldicarb sulfone	-0.57		47.5	55	40	4	0.28	-	-	1	-	-	-	-
atrazine		2.61	1.7	-	-	-	-	46.5	115	6.9	7	-	-	-	-
	deisopropyldeethyl atrazine	1.15		-	-	-	-	19.8	-	-	1	-	-	-	-
azocyclotin		5.3	5.36	0.004	-	-	1	0.04	-	-	1	0.16	-	-	1
	1,2,4-triazole	-0.58		-	-	-	-	-	-	-	-	22.5	-	-	1
	cyhexatin	5.39		0.003	0.0067	0.0013	6	0.0064	0.013	0.0002	2	-	-	-	-
benomyl		2.12		0.41	2.4	0.12	35	0.318	0.64	0.068	6	-	-	-	-
	carbendazim	1.52	4.2	0.625	4.5	0.024	22	0.405	0.64	0.11	4	-	-	-	-
	n-butylamine	0.97	10.8	268	268	32	3	-	-	-	-	-	-	-	-
bromoxynil		2.80	3.86	13.8	23	2.09	7	0.121	74	0.041	31	-	-	-	-
	4-hydroxybenzonitrile	1.6	7.97	22.6	-	-	1	15	-	-	1	-	-	-	-

Table C1. Ecotoxicity and physico-chemical property data for parent compounds and associated transformation products

Pesticide	Transformation product	log K_{ow}	pKa	Fish 96h LC_{50} (mg/L)				Daphnid 48h EC_{50} (mg/L)				Algae 72-96h EC/IC_{50} (mg/L)			
				Median	Max	Min	n	Median	Max	Min	n	Median	Max	Min	n
butylate		4.15	none	-	-	-	-	85.3	158.6	11.9	2	-	-	-	-
	diisobutylamine		10.9	-	-	-	-	35	-	-	1	-	-	-	-
	ethyl mercaptan		10.6	-	-	-	-	45.1	90	0.17	2	-	-	-	-
carbaryl		2.36	none	4.6	290	0.76	89	0.0072	16.8	0.0003	20	-	-	-	-
	1,2-dihydroxybenzene	0.88	9.45	9.06	9.22	3.5	4	1.66	-	-	1	-	-	-	-
	1,3-dihydroxybenzene	0.80	9.32	54.95	100	40	6	1.28	-	-	1	-	-	-	-
	1,4-dihydroxybenzene	0.59	10.9	0.14	0.638	0.044	8	0.21	0.29	0.13	2	-	-	-	-
	1-naphthol	2.85	9.34	4.18	4.63	3.57	4	-	-	-	-	-	-	-	-
	5-hydroxy-1,4-napthoquinonee	1.92		0.0432	0.088	0.034	13	-	-	-	-	-	-	-	-
chlomitrofen		5.09	none	-	-	-	-	-	-	-	-	0.0098	-	-	1
	4-nitrophenol	1.91	7.15	-	-	-	-	-	-	-	-	32	-	-	1
chlorpyrifos		4.99	none	0.041	2	0.0013	33	0.0006	0.0017	0.0001	5	-	-	-	-
	3,5,6-trichloro-2-pyridinol	3.21		1.5	-	-	1	-	-	-	-	-	-	-	-
	diethyl phosphorothioate		none	100	-	-	2	100	-	-	1	-	-	-	-
	oxalic acid		1.25	-	-	-	-	137	-	-	1	-	-	-	-
dazomet		1.4	none	1.35	16.2	0.16	6	6.11	11.9	0.31	2	1	-	-	1
	formaldehyde	0.35	13.3	41.4	149	1.41	33	10.2	29	0.2	4	-	-	-	-
	hydrogen sulphide		7.04	0.035	0.776	0.007	48	-	-	-	-	-	-	-	-
	methyl isothiocyanate	0.94	12.3	0.118	0.142	0.094	4	0.168	0.28	0.055	2	0.25	-	-	1
	methylamine	-0.57	10.6	711.27	-	-	1	433	702	163	2	-	-	-	-
	N,N'-dimethylthiourea	-0.24		-	-	-	-	16.5	-	-	1	-	-	-	-
DDT		6.91	none	0.0088	100	0.0012	83	0.002	125	0.0004	29	-	-	-	-
	DDD	6.02	none	-	-	-	-	0.0032	-	-	2	-	-	-	-
	DDE	6.51	none	0.07	4.4	0.042	3	0.035	-	-	1	-	-	-	-
	dicofol	5.02		0.51	2.9	0.124	8	-	-	-	-	-	-	-	-

Table C1. Ecotoxicity and physico-chemical property data for parent compounds and associated transformation products

Pesticide	Transformation product	log K_{ow}	pKa	Fish 96h LC_{50} (mg/L)				Daphnid 48h EC_{50} (mg/L)				Algae 72-96h EC/IC_{50} (mg/L)			
				Median	Max	Min	n	Median	Max	Min	n	Median	Max	Min	n
diazinon		3.81	none	0.53	10.3	0.02	52	0.001	0.002	0.0005	20	-	-	-	-
	diethyl phosphorothioate			100	-	-	2	100	-	-	1	-	-	-	-
	pyrimidinol			1200	-	-	1	-	-	-	-	-	-	-	-
	sulfotep	3.99	none	0.178	1	0.0016	5	0.0014	0.0025	0.0002	2	-	-	-	-
diclobenil		2.74	none	10.5	18	6	11	3.7	10	3.7	5	-	-	-	-
	2,6-dichlorobenzamide	0.77		275	469	235	3	856	-	-	1	-	-	-	-
	2,6-dichlorobenzoic acid	2.23	1.59	130	140	120	4	-	-	-	-	-	-	-	-
diclofop-methyl		4.62	nonee	0.335	21.9	0.15	16	-	-	-	-	-	-	-	-
	diclofop	4.58	3.43	21.9	-	-	1	-	-	-	-	-	-	-	-
diuron		2.68	none	8.55	300	1.95	18	1.4	12	1.4	5	0.0024	-	-	1
	3,4-dichloroaniline	2.69	2.97	8.06	13	1.94	18	0.79	13	0.1	19	3.7	4.8	2.2	4
fluquinconazole		3.24	none	-	-	-	-	-	-	-	-	0.046	-	-	1
	1,2,4-triazole	-0.58		-	-	-	-	-	-	-	-	72.5	-	-	1
	FBC 96912		none	-	-	-	-	-	-	-	-	0.24	-	-	1
fluometuron		2.23	none	37.25	96	2.96	12	9.9	-	-	1	-	-	-	-
	3-trifluoromethyl benzenamine	2.29	3.49	35	-	-	1	2.7	-	-	1	-	-	-	-
fluridone		1.87	12.3	8.1	22	4.2	19	-	-	-	-	-	-	-	-
	benzaldehyde	1.48	none	11.2	12.8	1.07	7	-	-	-	-	-	-	-	-
	m-(trifluoromethyl) benzaldehyde	2.47	none	0.92	1.13	0.76	3	-	-	-	-	-	-	-	-

Table C1. Ecotoxicity and physico-chemical property data for parent compounds and associated transformation products

Pesticide	Transformation product	log K_{ow}	pKa	Fish 96h LC_{50} (mg/L)				Daphnid 48h EC_{50} (mg/L)				Algae 72-96h EC/IC_{50} (mg/L)			
				Median	Max	Min	n	Median	Max	Min	n	Median	Max	Min	n
gamma-HCH		3.72	none	0.068	51	0.016	79	1.19	62	0.25	25	3.2	-	-	1
	1,2,3,4-tetrachlorobenzene	4.6	none	1.3	1.5	1.1	2	-	-	-	-	-	-	-	-
	1,2,3,5-tetrachlorobenzene	4.56	none	1.6	-	-	1	0.86	9.7	0.86	5	17.7	-	-	1
	1,2,4-trichlorobenzene	4.02	none	2.9	4.8	1.27	14	2.745	50	0.76	6	25.1	-	-	1
	1,2-dichlorobenzene	3.43	none	5.4	57	1.52	16	2.35	2.4	0.74	5	76.1	-	-	1
	1,4-dichlorobenzene	3.44	none	4	34.5	0.88	19	10.5	13.5	0.0007	7	-	-	-	-
	alpha-HCH	3.8	none	1.21	8	0.32	8	0.9	1	0.8	2	-	-	-	-
	beta-HCH	3.78	none	1.59	1.66	1.52	2	-	-	-	-	-	-	-	-
	delta-HCH	4.14	none	2.21	2.83	1.58	2	-	-	-	-	-	-	-	-
glyphosate		-4.1	0.8	125	7815.7	10	26	457	930	22	6	-	-	-	-
	formaldehyde	0.35	none	41.4	149	1.41	33	10.2	29	0.2	4	-	-	-	-
	methylamine	-0.57	none	711.27	-	-	1	433	702	163	2	-	-	-	-
malathion		2.36	none	0.242	25	0.002	60	0.0018	0.033	0.001	13	-	-	-	-
	diethyl fumarate		none	4.5	-	-	1	-	-	-	-	-		-	-
	diethyl maleate		none	18	-	-	1	-	-	-	-	-	-	-	-
	dimethyl phosphate			18	-	-	1	-	-	-	-	-	-	-	-
	fumaric acid	0.46		-	-	-	-	208	212	204	2	-	-	-	-
napropamide		3.36	none	12.7	30	9.4	6	-	-	-	-	-	-	-	-
	1-naphthol	2.85		4.18	4.63	3.57	4	-	-	-	-	-	-	-	-
parathion		3.83	none	0.75	10	0.018	41	0.0013	0.0072	0.0006	23	-	-	-	-
	4-aminophenol	0.04	10.5	12.6	24	1.2	2	1.1	-	-	1	-	-	-	-
	4-nitrophenol	1.91	7.15	26.2	78.9	3.8	21	8.4	36	4.7	8	-	-	-	-
	paraoxon	1.98	none	0.29	0.33	0.25	2	0.0002	-	-	1	-	-	-	-
phenmedipham		3.59	none	3	3.98	1.41	3	-	-	-	-	-	-	-	-
	3-toluidine	1.4	0.1	168	-	-	1	-	-	-	-	-	-	-	-

Table C1. Ecotoxicity and physico-chemical property data for parent compounds and associated transformation products

Pesticide	Transformation product	log K_{ow}	pKa	Fish 96h LC_{50} (mg/L)				Daphnid 48h EC_{50} (mg/L)				Algae 72-96h EC/IC_{50} (mg/L)			
				Median	Max	Min	n	Median	Max	Min	n	Median	Max	Min	n
propanil		3.07	none	8.6	14	2.3	7	5.75	11.4	1.2	4	-	-	-	-
	propionic acid	0.33	4.88	76.2	115	51	4	36.4	50	22.7	2	-	-	-	-
quinmerac		-1.11	3.96	-	-	-	-	-	-	-	-	149.25	250	48.5	2
	BH-518-2			-	-	-	-	-	-	-	-	700	-	-	1
	BH-518-5			-	-	-	-	-	-	-	-	150	-	-	1
quintozene		4.64	none	0.435	1.6	0.1	8	0.77	-	-	1	-	-	-	-
	2,3,4,5-tetrachlorophenol	3.88	6.35	0.41	0.441	0.205	3	-	-	-	-	-	-	-	-
	2,3,4,6-tetrachlorophenol	4.45	5.22	0.682	1.1	0.14	6	0.18	2.66	0.09	5	-	-	-	-
	2,3,4-trichlorophenol	3.8		-	-	-	-	1.1	-	-	1	-	-	-	-
	2,3,5,6-tetrachlorophenol	3.88	5.14	0.17	-	-	1	0.86	1.15	0.57	2	-	-	-	-
	2,3,5-trichlorophenol	3.84	5.8	-	-	-	-	1.1	-	-	1	-	-	-	-
	2,3,6-trichlorophenol	3.77	5.8	-	-	-	-	3.7	-	-	1	-	-	-	-
	2,4,5-trichlorophenol	3.72	7.4	0.902	3.06	0.0012	11	1.8	2.7	0.9	2	-	-	-	-
	2,4,6-trichlorophenol	3.68	6.23	2.8	9.7	0.32	17	2.2	6	0.27	7	-	-	-	-
	3,4,5-trichlorophenol	4.01	7.84	-	-	-	-	0.57	0.68	0.45	2	-	-	-	-
	3,5-dichlorophenol	3.62	8.18	-	-	-	-	1	-	-	1	-	-	-	-
	pentachloroanisole	5.45	4.7	0.65	-	-	1	0.027	-	-	1	-	-	-	-
	pentachlorophenol	5.12	4.7	0.233	3	0.018	92	0.88	4.59	0.038	48	-	-	-	-
	tetrachlorocatechol	4.29		1.27	-	-	1	-	-	-	-	-	-	-	-
rimsulfuron		-1.47	4.00	-	-	-	-	1000	1000	184	3	-	-	-	-
	IN-70942			-	-	-	-	137	178	95	2	-	-	-	-
tecnazene		4.38	none	0.37	-	-	1	-	-	-	-	-	-	-	-
	2,3,5,6-tetrachloroaniline	4.1	none	0.27	0.272	0.058	3	-	-	-	-	-	-	-	-
	2,3,5,6-tetrachlorthioanisole		none	0.21	-	-	1	-	-	-	-	-	-	-	-

Table C1. Ecotoxicity and physico-chemical property data for parent compounds and associated transformation products

Pesticide	Transformation product	log K_{ow}	pKa	Fish 96h LC_{50} (mg/L)				Daphnid 48h EC_{50} (mg/L)				Algae 72-96h EC/IC_{50} (mg/L)			
				Median	Max	Min	n	Median	Max	Min	n	Median	Max	Min	n
thiodicarb		1.7	none	2.01	2.65	1.21	4	0.049	0.053	0.027	3	-	-	-	-
	acetonitrile	-0.34	4.3	1020	1850	100	7	3600	-	-	1	-	-	-	-
	methomyl	0.6	none	1.45	32	0.48	44	0.0089	3.2	0.0076	6	-	-	-	-
triazamate		2.69	none	0.88	4.4	0.43	9	0.048	1.7	0.0035	9	2.2	240	0.3	5
	metabolite II	1.62		10	-	-	1	0.35	-	-	1	120	-	-	1
triclopyr		-0.45	3.97	7.5	148	1.1	5	-	-	-	-				
	3,5,6-trichloro-2-pyridinol	3.21		1.5	-	-	1	-	-	-	-				
trisulfusulfuron-methyl		0.96	4.4	730	760	71	3	669.5	1200	139	2	0.2785	0.62	0.037	4
	IN-D8526-2		2.65	139	-	-	1	324	-	-	2	177.5	-	-	1
zineb			none	93.6	180	7.2	2	20.5	40	0.97	2	18	-	-	1
	ethylenethiourea	-0.66		180	7500	7.2	3	26	40	0.97	3	1.8	-	-	1
	ethyleneurea			13000	-	-	1	5600	-	-	1	16	-	-	1

Table D1. Pesticides omitted from the prioritisation of transformation products used in agriculture in Great Britain and the reasons for their omission

Reason for prioritisation omission	Pesticides
Inorganic	bordeaux mixture, copper oxychloride, sodium chloride, sulphur, sulphuric acid
Undefined chemistry	anthracene oil, fatty acids, guazatine, natural plant extracts, tar oil, tridemorph
No significant environmental transformation products	amitrole, chlorpropham, clopyralid, cymoxanil, cyproconazole, difenoconazole, difenzoquat, dimethomorph, diquat, ethofumesate, henhexamid, fludioxonil, flutriafol, metconazole, paraquat, propamocarb hydrochloride
No quantifiable transformation product formation data	bentazone, bifenox, carbendazim, carboxin, chlorotoluron, chlorthal-dimethyl, cyanazine, dichlorprop, etridiazole, fentin acetate, fentin hydroxide, fosetyl-aluminium, maneb, MCPA, metazachlor, methyl bromide, metoxuron, monolinuron, napropamide, pentanochlor, thiabendazole, thiram, zineb
No environmental transformation products identified within the literature	2-chloroethylphosphonic acid, benazolin, bupirimate, carbetamide, carfentrazone-ethyl, chlormequat, chlormequat chloride, chloropicrin, choline chloride, clomazone, cyazofamid, dichlorophen, dichlorprop-P, diflufenican, dithianon, dodemorph, dodine, epoxiconazole, ethoprophos, fenpropimorph, fenuron, flamprop-M-isopropyl, formaldehyde, fosthiazate, fuberidazole, gamma-HCH, hymexazol, imazamethabenz-methyl, lenacil, mancozeb (zineb and maneb), MCPB, mepiquat, metalaxyl-M, metamitron, nicotine, ofurace, oxadiazon, oxadixyl, penconazole, peroxyacetic acid, picoxystrobin, prochloraz, propoxycarbazone-sodium, pyrazophos, pyrifenox, quinoxyfen, quizalofop-P-ethyl, sethoxydim, silthiofam, sodium monochloroacetate, spiroxamine, tebutam, thiacloprid, triadimenol, urea, zoxamide

Table D2. Pesticides omitted from the prioritisation of transformation products used in agriculture and amenity in California and the reasons for their omission

Reason for prioritisation omission	Pesticides
Inorganic	aluminium phosphide, ammonium sulphate, arsenic pentoxide, calcium carbonate, calcium hydroxide, calcium hypochlorite, carbon dioxide, chlorine, chromic acid, copper hydroxide, copper oxide (ous), copper oxychloride sulphate, copper sulphate (basic), copper sulphate (pentahydrate), cryolite, disodium octaborate tetrahydrate, kaolin, lime-sulphur, nitrogen (liquified), potassium biocarbonate, sodium chlorate, sodium hypochlorite, sulphur, sulphur fluoride, sulphuryl fluoride
Undefined chemistry	cottonseed oil, hydrotreated paraffinic solvent, mineral oil, modified phthalic glycerol alkd resin, molassess, orchex 796 oil, petroleum distillates, petroleum distillates (refined), petroleum oil (parafin based), petroleum oil (unclassified), vegetable oil
Adjuvant	alpha-(para-nonylphenol)-omega-hydroxypoly(oxyethylene), alpha-alkylaryl-omega-hydroxypoly(oxyethylene), alpha-octylphenyl-omega-hydroxypoly(oxyethylene), oleic acid (methyl ester), poly-1-para-menthene
No environmental transformation products identified within the literature	acrolein, azinphos-methyl, chloropicrin, chlorthal-dimethyl, cyanamide, fosetyl-aluminium, isopropyl alcohol, mancozeb, maneb, MCPA (dimethylamine salt), methyl bromide, naled, oxyfluorfen, paraquat dichloride, permethrin, phosmet, potassium n-methyldithio carbamate, propanil, propargite, s-metolachlor, sodium tetrathiocarbonate, tribufos, urea dihydrogen sulphate, ziram

Table D3. Transformation products considered during the prioritisation for Great Britain, compounds grouped by their data availability class and then ranked according to their risk index (Chapter 5)

Transformation product	Parent pesticide(s)	Data availability classification	Risk index
3,5,6-trichloro-2-pyridinol	chlorpyrifos / triclopyr	A	0.68984
thifensulfuron acid	thifensulfuron-methyl	A	0.06557
kresoxim-methyl acid	kresoxim-methyl	A	0.0187
O-desmethyl-thifensulfuron-methyl	thifensulfuron-methyl	A	0.00219
6-chloro-3-phenyl-pyridazin-4-ol	pyridate	A	0.00081
IN-A4098	metsulfuron-methyl	A	0.00069
DP-1	tepraloxydim	A	0.00005
DP-2	tepraloxydim	A	0.00004
aldicarb sulfoxide	aldicarb	A	0.00001
aldicarb sulfone	aldicarb	A	<0.00001
methomyl	thiodicarb	A	<0.00001
CGA-321113	trifloxystrobin	Bf	0.09058
carbendazim	thiophanate-methyl / benomyl	Bf	0.066
1,2,4-triazole	fluquinconazole / tebuconazole / tetraconazole / propiconazole / myclobutanil	Bf	0.04381
CL 153815	picolinafen	Bf	0.00113
diclofop acid	diclofop-methyl	Bm	2.65305
ethyl-m-hydroxyphenyl carbamate	desmedipham	Bm	0.00843
triazine amine A	tribenuron-methyl	Bm	0.00374
BTS 27919	amitraz	Bm	0.00353
DMST	tolylfluanid	Bm	0.00013
BTS 27271	amitraz	Bm	0.00009
FBC 96912	fluquinconazole	Bm	<0.00001
desmethylisoptoturon	isoproturon	Bp	0.61546
deethylatrazine	atrazine	Bp	0.2766
deisopropylatrazine	simazine / atrazine	Bp	0.20056
thiophene sulfonimide	thifensulfuron-methyl	Bp	0.10602
hydroxyatrazine	atrazine	Bp	0.10324
diaminochloroatrazine	atrazine	Bp	0.0836
2,4-D	2,4-DB	Bp	0.04434
tetrahydrophthalamide	captan	Bp	0.03893
HOE 35950	glufosinate-ammonium	Bp	0.01805
N-(1,1-dimethylacetonyl)-3,5-dichlorobenzamide	propyzamide	Bp	0.01781
BH518-2	quinmerac	Bp	0.01061
BH518-5	quinmerac	Bp	0.00769
aminomethylphosphonic acid	glyphosate	Bp	0.00544
2-(3,5-dichlorophenyl)-4,4-dimethyl-5-methyleneoxazoline	propyzamide	Bp	0.00333
saccharin	metsulfuron-methyl	Bp	0.00296
benalaxyl M2	benalaxyl	Bp	0.00106
RPA 406341	triticonazole	Bp	0.00094
3,5-dibromo-4-hydroxybenzamide	bromoxynil	Bp	0.00048
3,5-di-iodo-4-hydroxybenzamide	ioxynil	Bp	0.00041
3,6-dichlorosalicylic acid	dicamba	Bp	0.00039
benalaxyl M1	benalaxyl	Bp	0.00023
RP 30228	iprodione	Bp	0.00018
3-phenoxybenzoic acid	cypermethrin	Bp	<0.00001
3,5-di-iodo-4-hydroxybenzoic acid	ioxynil	Bp	<0.00001
3-phenoxybenzoic acid	tau-fluvalinate	Bp	<0.00001
RPA 407922	triticonazole	Bp	<0.00001
CGA 118 245	propiconazole	Bp	<0.00001
3,5-dibromo-4-hydroxybenzoic acid	bromoxynil	Bp	<0.00001

Table D3. Transformation products considered during the prioritisation for Great Britain, compounds grouped by their data availability class and then ranked according to their risk index (Chapter 5)

Transformation product	Parent pesticide(s)	Data availability classification	Risk index
propachlor oxanilic acid	propachlor	C	1.53945
propachlor ethane sulfonic acid	propachlor	C	0.88299
4-hydroxy-2,5,6-trichloroisophthalonitrile	chlorothalonil	C	0.72227
triazamate metabolite II	triazamate	C	0.36716
3,5,6-trichloro-2-methoxypyridine	chlorpyrifos / triclopyr	C	0.26540
4-(2,4-dichlorophenoxy)phenol	diclofop-methyl	C	0.25135
triazamate metabolite IV	triazamate	C	0.17616
omethoate	dimethoate	C	0.1087
triazamate metabolite III	triazamate	C	0.10578
fluzaifop acid	fluazifop-p-butyl	C	0.09033
diaminochlorotriazine	simazine	C	0.08733
methyl saccahrin	triflusulfuron-methyl	C	0.04872
3-methyl phosphinico-proprionic acid	glufosinate-ammonium	C	0.0394
hydroxysimazine	simazine	C	0.03532
N'-(3,4-dichlorophenyl)-N-methylurea	diuron	C	0.03002
Ro 17-3102	propaquizafop	C	0.02539
compound XII	fluazinam	C	0.00851
N-demethyl triazine amine B	triflusulfuron-methyl	C	0.0062
triazine amine B	triflusulfuron-methyl	C	0.0057
4-amino-3,5-dichloro-6-fluoromethoxypyridine	fluroxypyr	C	0.00396
N,N-bis demethyl triazine amine B	triflusulfuron-methyl	C	0.00359
methylisothiocyanate	metam-sodium	C	0.00262
HOE 101630	amidosulfuron	C	0.00248
2,4-dichlorophenol	2,4-D	C	0.00212
2,4-bis(isopropylamino)-6-hydroxy-s-triazine	prometryn	C	0.00183
malathion dicarboxylic acid	malathion	C	0.00164
4-amino-3,5-dichloro-6-fluoro-2-pyridinol	fluroxypyr	C	0.00162
2-amino-4,6-dihydroxypyrimidine	amidosulfuron	C	0.00088
2-ester-3-sulfonamide	thifensulfuron-methyl	C	0.00057
1-(6-chloro-pyridine-3-ylmethyl)-N-nitro guanidine	imidacloprid	C	0.00044
IN-D5803	metsulfuron-methyl	C	0.00025
decamethrinic acid	deltamethrin	C	0.00024
BF 500-3	pyraclostrobin	C	0.00024
anilino acid	tau-fluvalinate	C	0.00011
2-amino-4-isopropylamino-6-methylthio-s-triazine	prometryn	C	0.00008
malathion monocarboxylic acids	malathion	C	0.00007
CGA 180777	pymetrozine	C	0.00003
GS23199	pymetrozine	C	<0.00001
CGA 249257	pymetrozine	C	<0.00001
3-phenoxybenzoic acid	alpha-cypermethrin	C	<0.00001
CGA 359009	pymetrozine	C	<0.00001
3-phenoxybenzoic acid	zeta-cypermethrin	C	<0.00001
1-methyl-3-(4-isopropyl phenyl)-urea	isoproturon	D	3.45795
TCPSA	tri-allate	D	1.91577
3-carbamyl-2,4,5-trichlorobenzoic acid	chlorothalonil	D	0.98035
methiocarb sulfoxide	methiocarb	D	0.85099
bis (4-fluorophenyl)methyl silanol	flusilazole	D	0.59419
desethylterbuthylazine	terbuthylazine	D	0.58532
bitertanol benzoic acid	bitertanol	D	0.56804
methiocarb sulfoxide phenol	methiocarb	D	0.5106
3-[4-(2'-hydroxy-2'-propyl)-phenyl]-methyl urea	isoproturon	D	0.44333
3-cyano-2,4,5,6-tetrachlorobenzamide	chlorothalonil	D	0.40783
DEHA	atrazine	D	0.37691
deaminated diketo metribuzin	metribuzin	D	0.35128
diketo metribuzin	metribuzin	D	0.32648

Table D3. Transformation products considered during the prioritisation for Great Britain, compounds grouped by their data availability class and then ranked according to their risk index (Chapter 5)

Transformation product	Parent pesticide(s)	Data availability classification	Risk index
FOE sulfonic acid	flufenacet	D	0.31247
demethyl linuron	linuron	D	0.3071
4-chloro-2-methyl phenol	mecoprop-p / mecoprop	D	0.27057
DIHA	atrazine	D	0.26727
methiocarb sulfone phenol	methiocarb	D	0.2553
MHPC	phenmedipham	D	0.23087
SAS 9256	triazoxide	D	0.23068
methiocarb sulfone quinone	methiocarb	D	0.22693
FOE oxalte	flufenacet	D	0.21737
α,α,α-trifluoro-2,6-dinitro-N-propyl-p-toluidine	trifluralin	D	0.20207
triazamate metabolite IX	triazamate	D	0.19512
methylisothiocyanate	dazomet	D	0.19231
O-desmethyldimethoate	dimethoate	D	0.1772
3-carbamyl-1,2,4,5-tetrachlorobezoic acid	chlorothalonil	D	0.16862
tralkoxydim metabolite 8	tralkoxydim	D	0.1604
tralkoxydim metabolite 10	tralkoxydim	D	0.1536
propachlor sulfinylacetic acid	propachlor	D	0.15177
3-cyano-6-hydroxy-2,4,5-trichlorobenzamide	chlorothalonil	D	0.14901
tetraconazole acid	tetraconazole	D	0.14433
IN-KZ007	famoxadone	D	0.14214
hydroxypropachlor	propachlor	D	0.13582
2,2'-azoxybis (α,α,α-trifluoro-6-nitro-N-propyl-p-toluidine	trifluralin	D	0.13178
3-cyano-2,5,6-trichlorobenzamide	chlorothalonil	D	0.12548
5,6-dimethyl-2-dimethylamino-pyrimidin-4-ol	pirimicarb	D	0.12265
α,α,α-trifluoro-2,6-dinitro-p-cresol	trifluralin	D	0.11861
2-ethyl-7-nitro-5-(trifluoromethyl) benzimidazole	trifluralin	D	0.11421
5-chloro-3-fluoro-2-hydroxy-pyridine	clodinafop-propargyl	D	0.11413
DCVA	beta-cyfluthrin	D	0.10917
acetaldehyde	metaldehyde	D	0.10587
reference compound 2	azoxystrobin	D	0.10579
deisopropyl hydroxyatrazine	simazine	D	0.1048
5,6-dimethyl-2-methylamino-4-pyrimidin-4-ol	pirimicarb	D	0.10221
5,6-dimethyl-2-methylamino-pyrimidin-4-yl-dimethylcarbamate	pirimicarb	D	0.10221
α,α,α-trifluoro-5-nitro-4-propyl-toluene-3,4-diamine	trifluralin	D	0.09225
CGA 249287	cyprodinil	D	0.08728
O,O-dimethylphosphorothioic acid	dimethoate	D	0.08438
Ro 40-2724	propaquizafop	D	0.0788
SAS 9709	triazoxide	D	0.07689
[2,6-dinitro-4-(trifluoromethyl)phenyl]propylamine	trifluralin	D	0.07468
propachlor methyl sulfone	propachlor	D	0.07249
tralkoxydim metabolite 9	tralkoxydim	D	0.06932
BF 500-6	pyraclostrobin	D	0.0607
norlinuron	linuron	D	0.06032
triazamate metabolite VIII	triazamate	D	0.06004
bitertanol ketone	bitertanol	D	0.05979
methiocarb phenol	methiocarb	D	0.05673
azoxystrobin acid	azoxystrobin	D	0.05036
5-amino-4-chloro-3-(2H)-pyridazinone	chloridazon	D	0.04935
2-ethyl-7-nitro-1-propyl-5-(trifluoromethyl) benzimidazole	trifluralin	D	0.04393
RP 36221	iprodione	D	0.03804
R0 12-7124	fenpropidin	D	0.03455
R0 18-5445	fenpropidin	D	0.03455
4-fluoro-3-phenoxybenzoic acid	beta-cyfluthrin	D	0.03181
SN 320-1	tebuconazole	D	0.03108
SN 3678-7/A	tebuconazole	D	0.03108
SN 3678-7/B	tebuconazole	D	0.03108

Table D3. Transformation products considered during the prioritisation for Great Britain, compounds grouped by their data availability class and then ranked according to their risk index (Chapter 5)

Transformation product	Parent pesticide(s)	Data availability classification	Risk index
methiocarb metabolite A	methiocarb	D	0.02837
methiocarb sulfone	methiocarb	D	0.02837
norchloropropachlor	propachlor	D	0.02718
compound VII	fluazinam	D	0.02481
fomesafen amine	fomesafen	D	0.02355
Ro 16-1976	propaquizafop	D	0.023
T2SO	cycloxydim	D	0.02199
HOE 64619	glufosinate-ammonium	D	0.02125
RP 25040	iprodione	D	0.02119
compound VIII	fluazinam	D	0.01985
T2SO	cycloxydim	D	0.01787
2,4-dichloroanisole	2,4-D	D	0.0174
APMP	phenmedipham	D	0.0171
2,6-dichlorobenzamide	dichlobenil	D	0.01599
compound XV	lambda-cyhalothrin	D	0.01492
CONH2-fen	esfenvalerate	D	0.01409
DX-105	thiophanate-methyl	D	0.0137
FH-432	thiophanate-methyl	D	0.0137
CGA-373466	trifloxystrobin	D	0.01334
2-ethyl-7-nitro-1-propyl-5-(trifluoromethyl) benzimidazole-3-oxide	trifluralin	D	0.01318
reference compound 30	azoxystrobin	D	0.01246
fomesafen amino acid	fomesafen	D	0.01172
RE 54488	flurtamone	D	0.00989
tetraconazole alcohol	tetraconazole	D	0.00902
trifluoroethanoic acid	flurtamone	D	0.00897
2,6-dinitro-4-(trifluoromethylphenyl)amine	trifluralin	D	0.00879
compound 1a	lambda-cyhalothrin	D	0.0087
paraldehyde	metaldehyde	D	0.00847
1-(2,4-dichlorohenyl) ethan-1-ol	chlorfenvinphos	D	0.0084
2,4-dichloroacetophenone	chlorfenvinphos	D	0.0084
2,4-dichlorophenyl chloride	chlorfenvinphos	D	0.0084
2,4-dichlorophenyl)-ethan-1,2-diol	chlorfenvinphos	D	0.0084
2,4-dichlorophenyloxrane	chlorfenvinphos	D	0.0084
desethyl chlorfenvinphos	chlorfenvinphos	D	0.0084
salts or conjugates desethyl chlorfenvinphos	chlorfenvinphos	D	0.0084
2,4-dichloro-1-(1-hydroxyethyl) benzene	chlorfenvinphos	D	0.00804
1-(6-chloro-pyridine-3-ylmethyl)-2-imino-imidazolidine	imidacloprid	D	0.00646
triazolylacetic acid	tetraconazole	D	0.0064
methylaminosulfanilide	dichlofluanid	D	0.00623
CGA-62826	metalaxyl	D	0.0058
2,3,5,6-tetrafluoro-4-methylbenzoic acid	tefluthrin	D	0.00561
haloaniline	tau-fluvalinate	D	0.00561
4-(6-chloro-2-benzoxazolyloxy)phenol	fenoxaprop-p-ethyl	D	0.0056
2-N-(2,6-dimethylphenyl)-2-methoxyacetylamino propanoic acid	metalaxyl	D	0.00541
BTS 24868	amitraz	D	0.00491
T2SO2	cycloxydim	D	0.00458
6-chloro-nicotinic acid	imidacloprid	D	0.00451
1-(6-chloro-pyridine-3-ylmethyl)-N-nitro-2-imino-imidazolidine-5-ol	imidacloprid	D	0.00451
1-(6-chloro-pyridine-3-ylmethyl)-N-nitroso-2-imino-imidazolidine	imidacloprid	D	0.00451
reference compound 28	azoxystrobin	D	0.00434
PP890	tefluthrin	D	0.00393
TSO2	cycloxydim	D	0.00321
desphenyl-fenvalerate	esfenvalerate	D	0.00282
BH518-1	quinmerac	D	0.00271
BH518-4	quinmerac	D	0.00271
maleic acid	maleic hydrazide	D	0.00261

Table D3. Transformation products considered during the prioritisation for Great Britain, compounds grouped by their data availability class and then ranked according to their risk index (Chapter 5)

Transformation product	Parent pesticide(s)	Data availability classification	Risk index
maleimide	maleic hydrazide	D	0.00261
3-phenoxybenzaldehyde	cypermethrin / tau-fluvalinate	D	0.00254
(3,5-dichlorophenyl)-N-(2,3-dihydroxy-1,1-dimethylpropyl)carboxamide	propyzamide	D	0.00231
(3,5-dichlorophenyl)-N-(3-hydroxy-1,1-dimethyl-2-oxopropyl)carboxamide	propyzamide	D	0.00231
(3,5-dichlorophenyl)-N-(3-hydroxy-1,1-dimethylpropyl)carboxamide	propyzamide	D	0.00231
[2-(3,5-dichlorophenyl)-4,4-dimethyl-1,3-oxazolin-5-ylidene]methan-1-ol	propyzamide	D	0.00231
2-[(3,5-dichlorophenyl)carbonylamino]-2-methylpropanoic acid	propyzamide	D	0.00231
3-[(3,5-dichlorophenyl)carbonylamino]-3-methyl-2-oxobutanoic acid	propyzamide	D	0.00231
3-[(3,5-dichlorophenyl)carbonylamino]-3-methylbutanoic acid	propyzamide	D	0.00231
ionic form of asulam	asulam	D	0.0021
CCA	cypermethrin	D	0.00198
dintro octyl phenol	dinocap	D	0.00185
trinexapac acid	trinexapac-ethyl	D	0.00184
T2SO2	cycloxydim	D	0.00183
4'-OH-fen	esfenvalerate	D	0.00176
Cl-Vacid	esfenvalerate	D	0.00176
SD 50365	esfenvalerate	D	0.00176
RPA 406780	triticonazole	D	0.00169
ZK 512723	pyrimethanil	D	0.00169
dicarboxylic acid	tau-fluvalinate	D	0.00168
BF 500-5	pyraclostrobin	D	0.00162
490M0	kresoxim-methyl	D	0.00154
ketone metabolite	paclobutrazol	D	0.0015
DM-TM	tolclofos-methyl	D	0.00147
5-amino-4-chloro-2-methyl-2-hydropyridazin-3-one	chloridazon	D	0.00138
T1S	cycloxydim	D	0.00137
T1SO	cycloxydim	D	0.00137
DP-4	tepraloxydim	D	0.0013
RPA 404766	triticonazole	D	0.00126
CGA-357261	trifloxystrobin	D	0.00124
490M4	kresoxim-methyl	D	0.00115
fomesafen nitro acid	fomesafen	D	0.00115
2-(aminosulfonyl) benzoic acid	metsulfuron-methyl	D	0.001
benalaxyl acid	benalaxyl	D	0.00099
RPA 404886	triticonazole	D	0.00089
methomyl oxime	thiodicarb	D	0.00082
2,3,5,6-tetrafluoro-1,4-benzene dicarboxylic acid	tefluthrin	D	0.00073
CL 810 721	tebufenpyrad	D	0.00063
3-benzylbenzoic acid	esfenvalerate	D	0.00062
IN-B5685	metsulfuron-methyl	D	0.00059
conjugated form of asulam	asulam	D	0.00057
ph-CH3	tolclofos-methyl	D	0.00057
tefluthrin compound V	tefluthrin	D	0.00056
IN-D5119	metsulfuron-methyl	D	0.00055
IN-NC148	metsulfuron-methyl	D	0.00055
RPA 406203	triticonazole	D	0.00053
methyl-2-(aminosulfonyl)benzoate	metsulfuron-methyl	D	0.00048
DM-TMO	tolclofos-methyl	D	0.00047
2,6-dimethoxybenzoic acid	isoxaben	D	0.00047
RNH 0166	tolylfluanid	D	0.00042
RNH 0189	tolylfluanid	D	0.00042
RNH 0416	tolylfluanid	D	0.00042
3-(1-ethyl-1-methylpropyl)-4-hydroisoxazol-5-one	isoxaben	D	0.0004
3-(1-ethyl-1-methylpropyl)isoxazole-5-ylamine	isoxaben	D	0.0004
N-demethyl triazine amine A	tribenuron-methyl	D	0.00039
O-desmethyl metsulfuron	metsulfuron-methyl	D	0.00038

Table D3. Transformation products considered during the prioritisation for Great Britain, compounds grouped by their data availability class and then ranked according to their risk index (Chapter 5)

Transformation product	Parent pesticide(s)	Data availability classification	Risk index
demethyl isoxaben	isoxaben	D	0.00037
sulphanilamide	asulam	D	0.00033
O-demethyl triazine amine A	tribenuron-methyl	D	0.00027
dihydroxy triticonazole	triticonazole	D	0.00026
triticonazole metabolite 8	triticonazole	D	0.00026
M510F49	boscalid	D	0.00022
Ro 1-1374	fenoxycarb	D	0.00021
Ro 16-8797	fenoxycarb	D	0.00021
Ro 17-3192	fenoxycarb	D	0.00021
TMO	tolclofos-methyl	D	0.00017
N-methylpiperidine	mepiquat chloride	D	0.00013
piperidine	mepiquat chloride	D	0.00013
2-hydroxy-6-methoxybenzamide	isoxaben	D	0.0001
LS 860976	bromuconazole	D	0.00008
CGA-357276	trifloxystrobin	D	0.00007
TM-COOH	tolclofos-methyl	D	0.00007
ph-CH2OH	tolclofos-methyl	D	0.00006
ph-COOH	tolclofos-methyl	D	0.00006
TM-CH2OH	tolclofos-methyl	D	0.00006
TMO-CH2OH	tolclofos-methyl	D	0.00004
TMO-COOH	tolclofos-methyl	D	0.00004
malaoxon	malathion	D	0.00004
LS 860551	bromuconazole	D	0.00003
M1	imazaquin	D	0.00002
RPA 401527	bromuconazole	D	0.00002
CGA 294849	pymetrozine	D	<0.00001
pymetrozine metabolite IV	pymetrozine	D	<0.00001
CGA 215525	pymetrozine	D	<0.00001
CGA 319251	pymetrozine	D	<0.00001
cis-3-chloroallyl alcohol	1,3-dichloropropene	D	<0.00001
IN-JS940	famoxadone	D	<0.00001
trans-3-chloroallyl alcohol	1,3-dichloropropene	D	<0.00001
dimethyloxamic acid	oxamyl	E	2.28703
oxamyl oxime	oxamyl	E	2.28703
cis-3-chloroprop-2-enoic acid	1,3-dichloropropene	E	1.13026
trans-3-chloroprop-2-enoic acid	1,3-dichloropropene	E	1.13026
2-hydroxy terbutryn	terbutryn	E	1.07941
thiomethylol terbutryn	terbutryn	E	1.07941
3,5-dichloroaniline	vinclozolin/iprodione	E	0.81735
4-chlorobenzylamine	pencycuron	E	0.28594
4-chlorobenzylformamide	pencycuron	E	0.28594
IN-MN467	famoxadone	E	0.19126
FOE methyl sulfone	flufenacet	E	0.13586
FOE thioglycolate sulfoxide	flufenacet	E	0.13586
thiadone	flufenacet	E	0.13586
2,6-dinitro-3,4-xylidine	pendimethalin	E	0.13093
4-{(1-ethylpropyl)amino}-2-methyl-3,5-dinitro benzyl alcohol	pendimethalin	E	0.13093
4-{(1-ethylpropyl)amino}-3,5-dinitro-o-toluic acid	pendimethalin	E	0.13093
5-trifluoromethyl-pryid-2-one	fluazifop-p-butyl	E	0.10876
hydroxy-N-deethylated terbutryn	terbutryn	E	0.10794
thiomethylol deethylated terbutryn	terbutryn	E	0.10794
dimethylaminosulfanilide	dichlofluanid	E	0.07592
BF 500-7	pyraclostrobin	E	0.03372
4-hydroxy cypermethrin	alpha-cypermethrin / zeta-cypermethrin	E	0.0315

Table D3. Transformation products considered during the prioritisation for Great Britain, compounds grouped by their data availability class and then ranked according to their risk index (Chapter 5)

Transformation product	Parent pesticide(s)	Data availability classification	Risk index
cyano(3-hydroxyphenyl)methyl 3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate	alpha-cypermethrin / zeta-cypermethrin	E	0.0315
CGA-331409	trifloxystrobin	E	0.02942
CGA357262	trifloxystrobin	E	0.02942
NOA 413161	trifloxystrobin	E	0.02942
2-methyl-deaminated diketo metribuzin	metribuzin	E	0.02775
3-amino-deaminated metribuzin	metribuzin	E	0.02775
4-methyl-deaminated diketo metribuzin	metribuzin	E	0.02775
deaminated metribuzin	metribuzin	E	0.02775
1-(4,6-dimethoxypyrimidin-2-yl)-7-(trifluoromethyl)-1,3-dihydropyridino[2,3-d]pyrimidine-2,4-dione	flupyrsulfuron-methyl	E	0.02713
2-sulfamoyl-6-(trifluoromethyl)pyridine-3-carboxylic acid	flupyrsulfuron-methyl	E	0.02713
reference compound 10	azoxystrobin	E	0.02518
reference compound 20	azoxystrobin	E	0.02518
reference compound 3	azoxystrobin	E	0.02518
1-(2,4-dichlorophenyl)-2-imidazolylethan-1-ol	imazalil	E	0.02295
3,4-dichlorophenylurea	diuron	E	0.01236
deethyl ethirimol	ethirimol	E	0.00730
hydroxybutyl ethirimol	ethirimol	E	0.00730
4-fluoroaniline	carbosulfan	E	0.00447
acetonitrile	thiodicarb	E	0.00388
methomyl oxime sulfone	thiodicarb	E	0.00388
methomyl oxime sulfoxide	thiodicarb	E	0.00388
methomyl sulfone	thiodicarb	E	0.00388
methomyl sulfoxide	thiodicarb	E	0.00388
methyl 2-[(4-hydroxy-6-methoxypyrimidin-2-yl)amino]-6-(trifluoromethyl)pyridine-3-carboxylate	flupyrsulfuron-methyl	E	0.00271
amino-N-benzothiazol-2-yl-N-methylamide	methabenzthiazuron	E	0.00247
conjugated acetyl asulam	asulam	E	0.00092
conjugated acetyl sulphanilamide	asulam	E	0.00092
methylbenzenesulfonyl carbamate	asulam	E	0.00092
benzimidazole-2-ylamine	benomyl	E	0.00045
N-benzothiazol-2-yl(methylamino)carboxamide	methabenzthiazuron	E	0.00025
formaldehyde	daminozide	E	0.00001

Table D4. Transformation products considered during the prioritisation for California, compounds grouped by their data availability class and then ranked according to their risk index (Chapter 5)

Transformation product	Parent pesticide(s)	Data availability classification	Risk index
carbendazim	thiophanate-methyl	A	0.08
aldicarb sulfoxide	aldicarb	A	0.00001
RP 30228	iprodione	A	<0.00001
aldicarb sulfone	aldicarb	A	<0.00001
3,5,6-trichloro-2-pyridinol	chlorpyrifos	Bp	3.54859
tetrahydrophthalamide	captan	Bp	0.04328
aminomethylphosphonic acid	glyphosate	Bp	0.00748
3-phenoxybenzoic acid	cypermethrin	Bp	<0.00001
methylisothiocyanate	metam-sodium	C	2.67106
N'-(3,4-dichlorophenyl)-N-methylurea	diuron	C	1.83465
deisopropylatrazine	simazine	C	0.55712
malathion dicarboxylic acid	malathion	C	0.28916
4-hydroxy-2,5,6-trichloroisophthalonitrile	chlorothalonil	C	0.25575
omethoate	dimethoate	C	0.16653
diaminochlorotriazine	simazine	C	0.08146
hydroxysimazine	simazine	C	0.0586
methamidophos	acephate	C	0.0497
2,4-bis(isopropylamino)-6-hydroxy-s-triazine	prometryn	C	0.03064
molinate sulfoxide	molinate	C	0.02165
malathion monocarboxylic acids	malathion	C	0.01213
2,4-dichlorophenol	2,4-D	C	0.00719
hexamethyleneimine	molinate	C	0.00422
2-amino-4-isopropylamino-6-methylthio-s-triazine	prometryn	C	0.00131
desmethyl norflurazon	norflurazon	C	0.00098
EPTC sulfoxide	EPTC	C	0.00084
1-(6-chloro-pyridine-3-ylmethyl)-N-nitro guanidine	imidacloprid	C	0.00077
pyrimidinol	diazinon	D	6.69476
3,5,6-trichloro-2-methoxypyridine	chlorpyrifos	D	1.4461
2-hydroxy ethyl phosphonic acid	ethephon	D	0.71052
1-napthol	carbaryl	D	0.4105
3-carbamyl-2,4,5-trichlorobenzoic acid	chlorothalonil	D	0.34713
O-desmethyldimethoate	dimethoate	D	0.27147
ethylene	ethephon	D	0.16784
3-cyano-2,4,5,6-tetrachlorobenzamide	chlorothalonil	D	0.14441
hydroxyl-pyrimidinol	diazinon	D	0.13775
O,O-dimethylphosphorothioic acid	dimethoate	D	0.12927
deisopropyl hydroxyatrazine	simazine	D	0.11347
4-chlorobezoic acid	thiobencarb	D	0.10296
RP 36221	iprodione	D	0.08573
α,α,α-trifluoro-2,6-dinitro-N-propyl-p-toluidine	trifluralin	D	0.07142
3-carbamyl-1,2,4,5-tetrachlorobezoic acid	chlorothalonil	D	0.05971
3-cyano-6-hydroxy-2,4,5-trichlorobenzamide	chlorothalonil	D	0.05276
RP 25040	iprodione	D	0.04776
2,2'-azoxybis (α,α,α-trifluoro-6-nitro-N-propyl-p-toluidine	trifluralin	D	0.04658
3,5-dichloroaniline	iprodione	D	0.04549
3-cyano-2,5,6-trichlorobenzamide	chlorothalonil	D	0.04443
α,α,α-trifluoro-2,6-dinitro-p-cresol	trifluralin	D	0.04192
2-ethyl-7-nitro-5-(trifluoromethyl) benzimidazole	trifluralin	D	0.04037
2,4-dichloroanisole	2,4-D	D	0.03956

Table D4. Transformation products considered during the prioritisation for California, compounds grouped by their data availability class and then ranked according to their risk index (Chapter 5)

Transformation product	Parent pesticide(s)	Data availability classification	Risk index
α,α,α-trifluoro-5-nitro-4-propyl-toluene-3,4-diamine	trifluralin	D	0.0326
bensulide oxon	bensulide	D	0.02771
[2,6-dinitro-4-(trifluoromethyl)phenyl]propylamine	trifluralin	D	0.02639
S-methyl-N-hydroxythioacetimidate	methomyl	D	0.02558
DX-105	thiophanate-methyl	D	0.02208
FH-432	thiophanate-methyl	D	0.02208
CGA 249287	cyprodinil	D	0.01702
2-ethyl-7-nitro-1-propyl-5-(trifluoromethyl) benzimidazole	trifluralin	D	0.01553
cis-3-chloroallyl alcohol	1,3-dichloropropene	D	0.01465
1-(6-chloro-pyridine-3-ylmethyl)-2-imino-imidazolidine	imidacloprid	D	0.00747
malaoxon	malathion	D	0.00642
4-hydroxy-3,5-dinitro-benzenesulfonamide	oryzalin	D	0.00590
6-chloro-nicotinic acid	imidacloprid	D	0.00521
1-(6-chloro-pyridine-3-ylmethyl)-N-nitro-2-imino-imidazolidine-5-ol	imidacloprid	D	0.00521
1-(6-chloro-pyridine-3-ylmethyl)-N-nitroso-2-imino-imidazolidine	imidacloprid	D	0.00521
2-ethyl-7-nitro-1-propyl-5-(trifluoromethyl) benzimidazole-3-oxide	trifluralin	D	0.00466
2,6-dinitro-4-(trifluoromethylphenyl)amine	trifluralin	D	0.00311
2-ethyl-7-nitro-1-propyl-1H-benzimidazole-5-sulfonamide-3-oxide	oryzalin	D	0.00263
3,3'-azoxybis[4-(propylamino)-5-nitro] benzenesulfonamide	oryzalin	D	0.00176
3-phenoxybenzaldehyde	cypermethrin	D	0.00174
CCA	cypermethrin	D	0.00174
3,5-dinitro-4-(propylamino) benzenesulfonamide	oryzalin	D	0.00151
trans-3-chloroallyl alcohol	1,3-dichloropropene	D	<0.00001
cis-3-chloroprop-2-enoic acid	1,3-dichloropropene	E	9.83109
trans-3-chloroprop-2-enoic acid	1,3-dichloropropene	E	9.83109
o,p'-dichlorobenzophenone	dicofol	E	5.43847
2-chlorobenzoic acid	dicofol	E	5.43847
3-hydroxy-2,4-dichlorobenzophenone	dicofol	E	5.43847
2,4'-dichlorobenzhydrol	dicofol	E	5.43847
1,1-(p-chlorophenyl)-2,2-dichloroethanol	dicofol	E	5.43847
p,p'-dichlorobenzophenone	dicofol	E	5.43847
3-hydroxy-4,4'-dichlorobenzophenone	dicofol	E	5.43847
endosulfan sulphate	endosulfan	E	0.7836
3,4-dichlorophenylurea	diuron	E	0.67306
2,6-dinitro-3,4-xylidine	pendimethalin	E	0.00877
4-[(1-ethylpropyl)amino]-2-methyl-3,5-dinitro benzyl alcohol	pendimethalin	E	0.00877
4-[(1-ethylpropyl)amino]-3,5-dinitro-o-toluic acid	pendimethalin	E	0.00877

Table D5. Calculated indices for the top four transformation products with data availability classification A for Great Britain and California, data values used for the calculations were from Table 17 and 18 in Chapter 5

Transformation product	Parent pesticide(s)	A	F	P	E	RI
Great Britain						
3,5,6-trichloro-2-pyridinol [a]	chlorpyrifos/ triclopyr	-	-	-	-	6.90E-01
thifensulfuron acid	thifensulfuron-methyl	1.86E-03	4.91E-01	7.19E-01	6.60E-04	6.56E-02
kresoxim-methyl acid	kresoxim-methyl	3.53E-02	2.82E-01	7.53E-01	7.48E-03	1.87E-02
IN-A4098	metsulfuron-methyl	1.41E-03	1.64E-01	9.48E-02	2.00E-05	2.19E-03
California						
carbendazim	thiophanate-methyl	6.46E-03	4.26E-01	5.82E-01	1.60E-03	8.00E-02
aldicarb sulfoxide	aldicarb	1.63E-02	6.62E-01	3.45E-06	3.72E-08	1.24E-05
RP 30228	iprodione	6.02E-03	2.52E-03	1.87E-07	2.84E-12	1.42E-10
aldicarb sulfone	aldicarb	1.42E-02	7.87E-01	3.49E-14	3.89E-16	1.30E-13

[a] - multiple values of the A, F, P and E indices not provided