Evaluating the Use of Event Mean Concentration Models for the Management of Urban Drainage Systems

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Summary

This thesis has investigated the potential for simple pollution description techniques to be used within Integrated Catchment Models. The thesis proposes the use of an event mean concentration (EMC) as a measure which could be used to improve the assessment and design of solutions to manage the impacts of pollution on receiving water courses.

Processes and models proposed by previous research which predict storm water TSS concentrations in urban catchments have been presented and discussed. The most important considerations when developing a simple transferable TSS EMC storm water model have been identified as the inclusion of components which account for the build-up and wash-off processes which can be conceptualized using explanatory variables. In this respect, following analyses of a comprehensive TSS storm water quality data set collected in Australia, a new TSS EMC model which uses climatic and rainfall characteristic variables has been developed. Analysis of the model's calibration and validation results were compared with those made by existing TSS EMC models and showed that the model had significant predictive efficiency.

To understand the potential and practical application of the model to catchments other than where it was developed, the model has been calibrated and validated to a water quality data set generated by a complex deterministic sewer quality model, subsequently, it has been used to estimate observed TSS EMC's recorded at this catchment. Model calibration and validation results suggest that TSS EMC model accurately 'mimics' some of the water quality processes described by the complex model.

The simple EMC approach and associated uncertainty method presented in this work could be used to improve the application of the ICM process by offering practitioners and decision makers a new planning dimension; the interpretation of probabilistic results which could be used to improve the application and understanding associated with the ICM approach.

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List of Acronyms

BOD	Biological Oxygen Demand
CDT	Concentration Duration Threshold
CSO	Combined Sewer Overflow
DO	Dissolved Oxygen Concentration
EMC	Event Mean Concentration
EQO	Environmental Quality Objectives
EQS	Environmental Quality Standards
FIS	Fundamental Intermittent Standards
ICM	Integrated Catchment Management
NH_4	Ammonium
PDF	Probability Density Function
RQIM	River Quality Impact Model
RMSE	Root Mean Square Error
SMC	Site Mean Concentration
SRG	Stochastic rainfall generator
STO	Storm Tank Overflow
STQM	Sewage Treatment Work Model
SQM	Sewer quality model
SUDS	Sustainable Urban Drainage Systems
SWMM	Storm Water Management Model
TSR	Annual Time Series Rainfall
TSS	Total Suspended Solids

UDS	Urban Drainage System
WRC	Water Research Council
WWTW	Wastewater Treatment Works

Equations and Notation

The following equations list and respective notation is specific to each chapter in which it is presented:

Equation 3-1

$$\frac{\mathrm{dM}}{\mathrm{dt}} = \mathrm{Ps} - (\mathrm{K_1} * \mathrm{M})$$

Where:

M = the mass of deposit per surface unit (kg/ha)

Ps = the build-up factor (kg/ha.day)

K_1= the decay factor (0.08/day) default deduced from empirical calibration.

Equation 3-2

$$M_{max} = \frac{Ps}{K_1}$$

Where:

M_{max} = maximum surface mass available (kg/ha)

Ps = the build-up factor (kg/ha.day)

K_1= the decay factor (0.08/day) default deduced from empirical calibration.

Equation 3-3

$$M_0 = M_d e^{-K_1 NJ} + \frac{Ps}{K_1}(1 - e^{K_1 NJ})$$

Where:

M_0 = the mass of sediment at the end of the build-up period or the projected mass at the end of the timestep (kg/ha)

M_d = the initial mass of sediment deposit (kg/ha)

K_1= the decay factor (0.08/day) default deduced from empirical calibration

NJ = the duration of the dry weather period or timestep length (days)

P_s = the build-up factor (kg/ha.day).

Equation 3-4

$$PG_n(t) = \frac{((C + M * ND) * V_g}{1{,}000{,}000}$$

Where:

$PG_n(t)$ = dissolved pollutant mass at timestep t (kg)

C = initial pollutant concentration (mg/l)

M = gradient of linear accumulation (mg/l days^{-1})

ND = dry weather period or timestep length (days)

V_g = gully pot volume (m^3).

Equation 3-5

$$V_g = D_g * A$$

Where:

V_g = gully pot volume (m^3)

D_g = gully pot depth (m)

A = runoff area of the respective runoff surface for the gully pot under consideration (m^2).

Equation 3-6

$$\frac{dM}{dt} = K_a * M(t) - f(t)$$

Where:

$M(t)$ = mass of surface-deposit pollution per unit area (kg/ha) at time t

K_a = the erosion/dissolution factor related to rainfall intensity (-)

$f(t)$ = the pollutant flow at time t (kg/(ha).

Equation 3-7

$$Me(t) = k * f(t)$$

Where:

Me(t) = the mass of the pollutant dissolved or suspended pollutant (kg/ha) at time (t) per unit area.

k = linear reservoir coefficient (s^{-1})

f(t) = the pollutant flow at time t (kg/(ha.s).

Equation 3-8

$$f(0) = \frac{Fm(0)}{C * Ar}$$

Where:

$f(0)$ = initial TSS outflow (kg/(s.ha))

$Fm(0)$ = the TSS flow (kg/s)

C = proportion of sub-catchment area that is impermeable (-)

Ar = sub-catchment area (ha).

Equation 3-9

$$Kpn = C_1(IMKP - C_2)^{C_3} + C_3$$

Where:

Kpn = Potency factor (-)

IMKP = maximum rainfall intensity over a 5-minute period (mm/hr)

C_1, C_2, C_3 = coefficients (mm/hr).

Equation 3-10

$$fn(t) = kpn * fm(t)$$

Where:

fn(t) = pollutant flow (kg/(s.ha) at time t

kpn = potency factor (-)

fm(t) = TSS flow at time t (kg/(s.ha).

Equation 3-11

$$\frac{dM}{dt} = -K_a M(t)$$

Where:

M = erosion rate (kg/(ha.s))

K_a = rainfall erosion coefficient (-)

M(t) = erosion rate at time t (kg/(ha)).

Equation 3-12

$$E = M(t) * \frac{(1 - e^{K_d dt})}{dt}$$

Where:

E = erosion rate (kg/(ha.s))

M(t) = erosion rate at time t (kg/(ha.s))

K_d = erosion coefficient (-).

Equation 3-13

$$B = \frac{(P_s - K_1 * M(t))dt}{86400}$$

Where:

B = surface build-up (kg/ha)

P_s = build-up coefficients (-)

K_1 = linear reservoir coefficient (-)

M(t) = erosion rate at time t (kg/(ha.s))

86400 (seconds in 24 hours).

Equation 3-14

$$M(t+dt) = M(t)e^{-K_a dt} + B$$

Where:

M(t) = erosion rate at time t (kg/(ha.s))

K_a = rainfall erosion coefficient (-)

B = surface build-up (kg/s).

Equation 3-15

$$\frac{dM_e}{dt} = E - f(t)$$

Where:

M_e = the mass in solution per unit area (kg/ha)

E = erosion rate (kg/(ha.s))

f(t) = TSS flow per unit of active surface at time t (kg/(ha)).

Equation 3-16

$$f(t+dt) = f(t)e^{\frac{-dt}{k}} + \left(1 - e^{\frac{-dt}{k}}\right) + (1 - e^{-k_a dt})M(t)/dt$$

Where:

f(t) = TSS flow per unit of active surface (kg/(s.ha))

k = linear reservoir coefficient (-)

k_a = rainfall erosion coefficient (-)

M(t) = the mass of surface-deposit pollution (kg/ha).

Equation 3-17

$$Fm(t) = C * A_r * f(t)$$

Where:

$Fm(t) =$ TSS outflow per sub-catchment at time t (kg/s)

C = the proportion of sub-catchment area that is impermeable (-)

Ar = the sub-catchment area (ha)

f(t) = TSS flow per unit of active surface at time t (kg/(s.ha)).

Equation 3-18

$$Fn(t) = kpn * C * Ar * f(t)$$

Where:

Fn(t) = the attached pollutant flow (kg/s)

kpn = potency factor (-)

C = the proportion of sub-catchment area that is impermeable (-)

Ar = the sub-catchment area (ha)

f(t) = TSS flow per unit of active surface at time t (kg/(s.ha)).

Equation 3-19

$$P_n = F_n(t + dt) * dt + PG_n(t)$$

Where:

P_n = total pollutant mass (kg)

$F_n(t + dt)$ = dissolved pollutant inflow (kg/s)

dt = timestep (s)

$PG_n(t)$ = pollutant in gully at time t (kg).

Equation 3-20

$$F_n(t+d) = \frac{Q(t+dt)}{(Q(t+dt)+\frac{V_g}{dt})} * \frac{P_n}{dt}$$

Where:

$F_n(t + dt)$ = dissolved pollutant inflow (kg/s)

Q (t + dt) = runoff from road surface at time t (m^3/s)

P_n = total pollutant mass (kg)

dt = timestep (s)

V_g= volume of gully (m^3).

Equation 3-21

$$PG_n(t+dt) = P_n - F_n(t+dt) * dt$$

Where:

$PG_n(t + dt)$ = pollutant in gully at timestep (kg)

P_n = total pollutant mass (kg)

dt = timestep (s)

$F_n(t + dt)$ = dissolved pollutant inflow (kg/s)

Note in current model no dissolved pollutant enters the gully pot from the road surface therefore $F_n(t + dt)$ input to the P_n equation is always zero.

Equation 3-22

$$\frac{dc}{dt} + u\frac{dc}{dx} = 0$$

Where:

c = concentration (kg/m^3)

u = the flow velocity (m/s) (obtained from the hydraulic simulation)

t = time (s)

x = the spatial co-ordinate (m).

Equation 3-23

$$C_v = J\left(\frac{W_e R}{A}\right)^{\alpha}\left(\frac{d_{50}}{R}\right)^{\beta}\partial_c^{\gamma}\left\{\frac{|\mu|}{\sqrt{g(s-1)R}} - K\partial_c^{\gamma}\left(\frac{d_{50}}{R}\right)^{\epsilon}\right\}^{m}$$

Where:

C_v = non-dimensional carrying capacity (-)

W_e = the effective bed width (m)

R = hydraulic radius of flow (m)

A = cross sectional area of the flow (m^2)

d_{50} = average sediment particle size (m)

u = flow velocity (m/s)

$g =$ acceleration due to gravity (m/s^2)

s = specific gravity of sediment particles (-)

∂_c = the composite friction factor, calculated using the Colebrook-White formula as described in Voogt, van Rijn and van den Berg, (1991)

$J, \alpha, \beta, \delta,\ K,\ \gamma,\ \varepsilon,\ m,$ = coefficients dependent on the dimensionless grain size D_{gr}.

Equation 3-24

$$D_{gr} = d_{50}\left(\frac{g(s-1)}{\mu^2}\right)^{\frac{1}{3}}$$

Where:

D_{gr} = grain size (-)

d_{50} = the average sediment particle size (m)

μ = the kinematic viscosity of water (m^2/s)

g = the acceleration due to gravity (m/s^2)

s = the specific gravity of the sediment fraction (-).

Equation 3-25

$$C_{max} = C_v \rho s$$

Where:

C_{max} = maximum carrying concentration (kg/m^3)

C_v = non-dimensional carrying capacity (-)

ρ = density of fluid (kg/m^3)

s = the specific gravity of the sediment fraction (-).

Equation 3-26

$$V_E = \sqrt{\sum_{t=0}^{t=n} \left(M_{i,t} - EMC_i\right)^2}$$

Where:

V_E = mean variation between the optimum EMC and the measured data for each event (mg/l)

$M_{i,t}$ = the measured parameter during spill event i at time *t* (mg/l)

EMC_i = EMC for spill event i (mg/l).

Equation 3-27

$$V_i = \sqrt{\sum_{t=0}^{t=n} \left(M_{i,t} - P_{i,t}\right)^2}$$

Where:

V_i = Minimum achievable variance between observed and predicted quality parameters for each event (mg/l)

P_{it} = the predicted value of the concentration parameter during event *i* at time *t* (mg/l)

$M_{i,t}$ = the measured parameter during spill event i at time *t* (mg/l).

Equation 4-1

$$W = W_0(1 - e^{-KIt})$$

Where:

W_t = transported sediment load after time t (g/m^2)

W_0 = Initial load of material on surface (g/m^2)

K = Calibration parameter (mm^{-1})

I = Rainfall Intensity (mm/hr)

t = time (hr).

Equation 4-2

$$F_W = \frac{W}{W_0} = C_f(1 - e^{-KIt)}$$

Where:

F_w = Fraction of wash-off (-)

W = Weight of material mobilized (g/m^2)

W_0 = Initial mass of material on surface (g/m^2)

C_f = Capacity factor (-)

K = Calibration parameter (mm^{-1})

I = Rainfall Intensity (mm/hr)

t = time (hr).

Equation 4-3

$$\tilde{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$$

Where

for each observation x_i (mg/l),

$\tilde{x}$ = the mean of the observed variable (mg/l)

n = the number of observations in the data set.

Equation 4-4

$$SD = \sum_{i=1}^{n} \sqrt{\frac{(x_i - \tilde{x})^2}{n}}$$

Where:

for each observation x_i,

$\tilde{x}$ is the mean of the observed variable and n is the number of observations in the data

SD = standard deviation (mg/l)

$\tilde{x}$ = the mean of the observed variable (mg/l)

n = the number of observations in the data set.

Equation 4-5

$$\frac{dEMC}{dX} = \frac{b_1}{X}(X \leq \lambda) + \frac{b_3}{X^2}(X > \lambda)$$

Where:

EMC = TSS EMC (mg/l)

X = Rainfall Depth (mm) * Antecedent dry weather period (days)

λ = threshold value of X separating the two behaviors of EMC values

b_1 and b_3 = model calibration parameters (mg/l).

Equation 4-6

$$EMC = [(b_1 \ln(X) + b_2)(X \leq \lambda)] + \left[\left(\frac{b_3}{X} + b_4\right)(X > \lambda)\right]$$

Where:

EMC = TSS EMC (mg/l)

X = Rainfall Depth (mm) * Antecedent dry weather period (days)

λ = the threshold value of X separating the two behaviors of EMC values

b_1, b_2, b_4 and b_3 = model parameters (mg/l).

Equation 4-7

$$E = 1 - \frac{\sum_{i=1}^{n}(M_i^{obs} - M_i^{model})^2}{\sum_{i=1}^{n}(M_i^{obs} - \bar{M}_I)^2}[-\infty|1]$$

Where:

For each observation M_i,

E = Nash-Sutcliffe co-efficient

M^{obs} = Observed TSS EMC value for n data records (mg/l)

M^{model}= Simulated TSS EMC for n data records (mg/l)

$\bar{M}_I$= Mean TSS EMC of observed data records (mg/l).

Equation 5-1

$$\frac{dC}{dt} = -kC$$

Where:

C = Pollutant concentration (mg/l)

k = the decay constant (s^{-1}).

Equation 5-2

$$\frac{1}{C}\frac{dC}{dt} = -k$$

Where:

C = Pollutant concentration (mg/l)

k = the decay constant (s^{-1}).

Equation 5-3

$$\frac{1}{C}\,dc = \,-k\,dt$$

Where:

C = Pollutant concentration (mg/l)

k = the decay constant (s^{-1}).

Equation 5-4

$$\int_0^{\infty}\frac{1}{C}\,dC = \int_0^{\infty}-k\,dt$$

Where:

C = Pollutant concentration (mg/l)

k = the decay constant (s^{-1}).

Equation 5-5

$$lnC + c_1 = -k\,t + \;c_2$$

Where:

C = pollutant concentration (mg/l)

k = the decay constant (s^{-1})

c_1 and c_2 = arbitrary constants.

Equation 5-6

$$lnC = -kt + c_3$$

C = pollutant concentration (mg/l)

k = the decay constant (s^{-1})

c_3 = arbitrary constant (-)

Equation 5-7

$$e^{(\ln C)} = e^{(-kt+c_3)}$$

Where:

C = pollutant concentration (mg/l)

k = the decay constant (s^{-1})

c_3 = arbitrary constant (mg/l).

Equation 5-8

$$C = e^{-kt+c_3}$$

Where:

C = pollutant concentration (mg/l)

k = the decay constant (s^{-1})

c_3 = arbitrary constant (mg/l).

Equation 5-9

$$C = e^{-kt}e^{c_3}$$

Where:

C = pollutant concentration (-)

k = the decay constant (s^{-1})

c_3 = arbitrary constant (mg/l).

Equation 5-10

$$C(t) = c_4e^{-kt}$$

Where:

C = pollutant concentration at time t (mg/l)

k = the decay constant (s^{-1})

c_4 = arbitrary constant (mg/l).

Equation 5-11

$$C(0) = C_0 = c_4 e^{-k\,0} = c_4 e^0 = c_4$$

C = pollutant concentration (mg/l) at time (0)

k = the decay constant (s^{-1})

c_4 = arbitrary constant (mg/l).

Equation 5-12

$$C_{(t)} = C_0 e^{-kt}$$

Where:

$C_{(t)}$ = the concentration of pollutant at time t (mg/l)

C_0 = the initial concentration at time (0) (mg/l)

k = the decay coefficient (s^{-1}).

Equation 5-13

$$C_{mean} = \frac{A_0}{T}$$

Where:

C_{mean} = TSS EMC (mg l^{-1})

A_0 = Total mass over duration of event (mg s l^{-1})

T = duration of the wash-off event (s).

Equation 5-14

$$A_O = A_I = \int_0^T C_0 e^{-kT} = \frac{C_0}{-k} e^{-kT} - \frac{C_0}{-k} e^{-k0}$$

Where:

C_0 = TSS EMC at time (0) (mg/l)

A_0 = Total mass over duration of event (mg s l^{-1})

A_I = Total mass over duration of event (mg s l^{-1})

T = duration of the wash-off event (s)

k = the decay coefficient (s^{-1}).

Equation 5-15

$$C_{mean} = \frac{1}{T}\,\frac{c_0}{-k}\left(e^{-kT} - 1\right)$$

Where:

C_{mean} = TSS EMC (mg/l)

C_0 = Initial TSS concentration (mg/l)

k = the decay coefficient (s^{-1})

T = duration of the wash-off event (s).

Equation 5-16

$$RMSE = \sum_{i=1}^{n}\left[\frac{Cpred_i - Cmeasured_i}{n}\right]^{\frac{1}{2}}$$

Where:

for each data point C_i,

RMSE = root-mean-square error (mg/l)

C_{pred} = TSS EMC (mg/l) predicted by the specific model formulation under analysis

$C_{measured}$ = observed TSS EMC (mg/l)

n = number of observations in the data set.

Equation 5-17

$$C_0 = a * \ln(ADWP) + b$$

Where:

C_0 = Initial TSS (mg L^{-1}) concentration at time (0)

$ADWP$ = antecedent dry weather period (s)

a and b = calibration parameters (mg L^{-1}).

Equation 5-18

$$k = c * e^{d*AGI5}$$

k = decay coefficient (s^{-1})

$AGI5$ = average rainfall intensity (mm/s)

c = calibration parameter (s^{-1})

d = calibration parameter (-).

Equation 5-19

$$C_{mean} = \frac{1}{T}\frac{a * \ln(ADWP) + b}{c * e^{d*AGI5}}(e^{-c*e^{d*AGI5}*T} - 1)$$

Where:

C_{mean} = TSS EMC (mg/l)

T = duration of the wash-off event (s)

$AGI5$ = average rainfall intensity (mm/hr)

$ADWP$ = antecedent dry weather period (hr)

a = calibration parameter (mg/l)

b = calibration parameter (mg/l)

c = calibration parameter (s^{-1})

d = calibration parameter (-)

Equation 5-20

$$S_{sc} = \frac{\sum_{i=1}^{NF} SC_i}{NF}$$

Where:

S_{sc} = sensitivity index value

NF = the number of input parameters

SC_i = the sensitivity index of parameter i.

Equation 5-21

$$y = \left[\frac{\sum_{i=1}^{NF} SC_{i_{n_k-1}} - \sum_{i=1}^{NF} SC_{i_{n_k}}}{NF}\right]$$

Where:

S_{sc} = sensitivity index value

NF = the number of input parameters

SC_i = the sensitivity index of parameter i

n_k = the number of simulations.

Equation 5-22

$$Residual\ Error_i = Cpredicted_i - Cmeasured_i$$

Where:

for the event *i*,

$Residual\ Error$ = model residual error (mg/l)

$C_{predicted}$ = the model prediction of TSS EMC (mg/l)

C_{measured} = the measured TSS EMC (mg/l).

Equation 5-23

$$\frac{Cpredicted_i}{Cmeasured_i} = Cratio_i$$

Where:

for the event *i*,

$Cratio$ = ratio of error (-)

$C_{predicted}$ = the model prediction of TSS EMC (mg/l)

C_{measured} = the measured TSS EMC (mg/l).

Equation 5-24

$$Bin\ Size = 2 * \frac{IQR(x)}{\sqrt[3]{n}}$$

Where:

$Bin\ Size$ = number of bins

IQR = the Interquartile range of the data (x)

n = the number of observations.

Equation 5-25

$$y = f(x \mid \mu, \sigma) = \frac{1}{x\sigma\sqrt{2\pi}} e^{\frac{-(\ln x - \mu)^2}{2\sigma^2}}$$

Where:

μ = location parameter

σ = scale parameter

π = Pi (~3.142)

Equation 5-26

$$F(x|\mu,\sigma) = \frac{1}{\sigma\sqrt{2\pi}} \int_0^x \frac{e^{\frac{-(\ln(t)-\mu)^2}{2\sigma^2}}}{t} dt$$

Where:

μ = location parameter

σ = scale parameter

π = Pi (~3.142).

Equation 6-1

$$\frac{n+1}{m} = Return\ period$$

Where:

n = the number of years of data

m = the number of occurrences of the event under study.

Equation 6-2

$$YR = \left(\frac{SAAR}{M5-60}\right) * R$$

Where:

SAAR is the annual average rainfall (mm)

M5-60 = the 5-year 60-minute rainfall event (mm)

R = the rainfall ratio (-).

Chapter 1. Introduction

1.1 Background and motivation of research

Access to clean water is an integral part of any successful and thriving human society. Streams, rivers, lakes and wetlands not only serve as potential raw sources of water, but also provide amenity, recreational value and are home to an abundance of flora and fauna. Drainage systems are necessary in urban areas to manage the interaction between human activity and the natural water cycle. Drainage systems are commonly required to handle two types of water that occur from anthropogenic activity; wastewater and storm water. Wastewater is derived from previously supplied potable water which has become adversely affected after domestic and industrial usage. Storm water is precipitation runoff which has fallen on the urban area. Wet weather conditions can lead to an exceedance related to a drainage systems capacity, subsequently, organic and in-organic matter carried within storm and wastewater flows can be released into the aquatic environment, these intermittent forms of discharge are a significant threat to the chemical and ecological health of receiving water bodies (European Environment Agency, 2012).

The European environment agencies report concerning the current status of water bodies across Europe estimated that only 52% of such bodies were set to reach the desired chemical and ecological status; defined as ‘good’, by the year 2015 (European Environment Agency, 2012). With world population numbers expected to continue increasing through the century and the number of people living within urbanised areas projected to rise from approximately 54% to 66%, it is expected that by the year 2050, an additional 2.5 billion people could be living in cities across the globe (United Nations World Water Assessment Programme, 2015). Urbanisation transforms natural drainage areas into hard standing surfaces which increases volumes of runoff in wet weather conditions, coupled with an increasingly uncertain climate and the higher wastewater and storm water loads associated with future anthropologic activity, water management bodies face significant challenges if they are to restore, maintain and protect water body health (Butler and Davies, 2010; and United Nations World Water Assessment Programme, 2015).

Water management bodies endeavour to manage the negative impacts of intermittent discharges from drainage systems by implementing a wide range of solutions across the drainage network. Solutions can range from traditional capital schemes such as network storage capacity upgrades, to more operationally based schemes such as the implementation of real-time-control systems or sustainable urban drainage systems (SUDS) (Butler and Davies, 2011). The design and success of such schemes is fundamentally underpinned by an ability to simulate and thus understand flow hydraulics and water quality behaviour throughout the system, mathematical models are commonly used provide this understanding (Ellis and Marsalek, 1996).

Catchments can be considered as explicit geographical areas in which a human population lives. A catchments respective drainage system can be conceptualised into different interconnected components; sewerage networks, surface water networks, wastewater treatment works and receiving water bodies into which all water derived from a catchment is discharged. Historically, each component of a catchment drainage system was managed and thus modelled alone; however, under the guidance of the Water Framework Directive, an integrated approach, one whereby the aforementioned components and respective models are considered as one is now necessary to deliver holistically orientated schemes which can account for both current and future environmental pressures, this relatively recent approach is defined as Integrated Catchment Management (ICM) (Lerner *et al.*, 2011). Whilst it is commonly accepted that the ICM approach is capable of coping with the requirements of the WFD, with such a wide range of computational models available to operators, and the new challenges this integrated approach to drainage modelling presents, the most effective and efficient means of delivering ICM are yet to be agreed (Freni, Mannina and Viviani, 2009).

A mathematical model of any catchments drainage system can be considered as a quantitative, objective, rational means of processing information to predict the systems future behaviour (Butler and Davies, 2011). The behaviour of wastewater and storm water within a catchment is influenced by a wide range of complex chemical, physiochemical, biological, ecological and physical processes. If the complexity of a model can be considered to increase with the number of processes modelled and the temporal and spatial scales at which these processes are simulated, and deterministic models are those which do not account for any random variation between mathematical relationships, then at present, the use of complex deterministic models to deliver the ICM approach is frequent and widespread (Freni *et al.*, 2008). This is in part due to the previous piecemeal approach to drainage modelling, but also due of a 'perceived' increase in modelling result accuracy associated with modelling individual processes in interlinked catchment dynamics at high temporal and spatial scales (Ashley, Hvitved-Jacobsen and Bertrand-Krajewski, 1999; Jakeman and Letcher, 2003; Hamilton *et al.*, 2015).

Simulating water quality behaviour within an integrated catchment model can be a computational demanding process. This is due to the computation power required to solve complex algorithms, as a result, model simulation times can become large. This length of time can become prohibitive for carrying out multiple simulations, thus impeding model calibration, uncertainty analyses, scenario testing and solution optimisation. Uncertainty analyses, scenario testing and solution optimisation can be dependent on the ability to run large numbers of simulations over a range of different modelling conditions (Mannina and Viviani, 2009). This length of time can become increasingly prohibitive as the numbers of sub-models exchanging information within an integrated model increases (Voinov and Shugart, 2013).

Because many water quality processes are not yet fully understood, can be dependent on model inputs and model parameters which are difficult to accurately quantify or may be subject to natural variability, the levels of uncertainty associated with water quality modelling is said to be high (Willems, 2010; Vezzaro *et al.*, 2012; Bach *et al.*, 2014). For this reason in an industrial context in which investment decisions regarding urban pollution management solutions are made by complex deterministic water quality models within integrated modelling approaches, there is a need to deal explicitly with uncertainty in water quality models (Pappenberger *et al.*, 2006).

As an alternative to deterministic models, various research groups have developed 'stochastically' based water quality modelling techniques capable of predicting pollutant loads and concentrations (Bach et al., 2010b and Daly et al., 2014). Stochastic modelling approaches consider some of the natural variability associated with water quality processes via the application of probability theory to variables and parameter values within a model. These techniques are dependent on the ability to run a model multiple times over various model input and parameter states. They are more readily applicable to 'simple' models, where run times are low, as oppose to complex, detailed, computationally expensive models widely used in the water industry (Obropta and Kardos, 2007a).

The successful application of simple modelling approaches can be reliant on data for catchment specific parameter calibration. In most practical cases, water quality data are extremely limited, consequently, due to the costs associated with calibrating simple models, their potential role within the integrated urban drainage modelling setting is yet to be fully evaluated (Bach *et al.*, 2014).

The implications of using simple water quality models that utilise stochastic techniques within the ICM process are that practitioners can increase the speed of urban drainage solution scenario testing, quantify the uncertainty associated with these model predictions and ultimately add knowledge to the design solution process through optimisation (Vezzaro *et al.*, 2013). Advancements in knowledge surrounding the delivery of the ICM will serve to aid the development of cost-effective solutions designed to manage the detrimental impacts of urban pollution on the water environment, of great benefit to engineering practitioners, the research community and the wider public.

1.2 Aims

This thesis tackles a relevant issue in integrated catchment modelling; the availability of water quality predictions for combined sewer overflows. The mechanistic models incorporated in state-of-the-art complex water quality models require significant, often excessive, computational efforts; thus, this work aims to explore and develop different computational methods capable of predicting combined sewer overflow water quality. The implications of the work are determining the impact on a river of pollution discharged via combined sewer overflows.

1.3 Objectives

The objectives of the thesis are as follows:

1. Study existing water quality modelling methods utilised in the protection and management of the negative impacts caused by urban discharges. Identify which methods are of importance and how current prediction techniques could be improved through water quality model simplification and uncertainty analyses. Identify a suitable method by which modelling complexity could be reduced.
2. Analyse the effects of reducing model complexity within an integrated model using case study data.
3. Evaluate and understand the implications associated with reducing model complexity within an integrated model, subsequently provide recommendations to aid the development of a novel simplified modelling technique.
4. Develop a new model with respect to the outcome of objectives 2 and 3.
5. Study the implications associated with the application and transferability of the new model.

1.4 Thesis Structure

Figure 1-1 shows a schematic outline of the research carried out and the way it is been presented throughout the thesis.

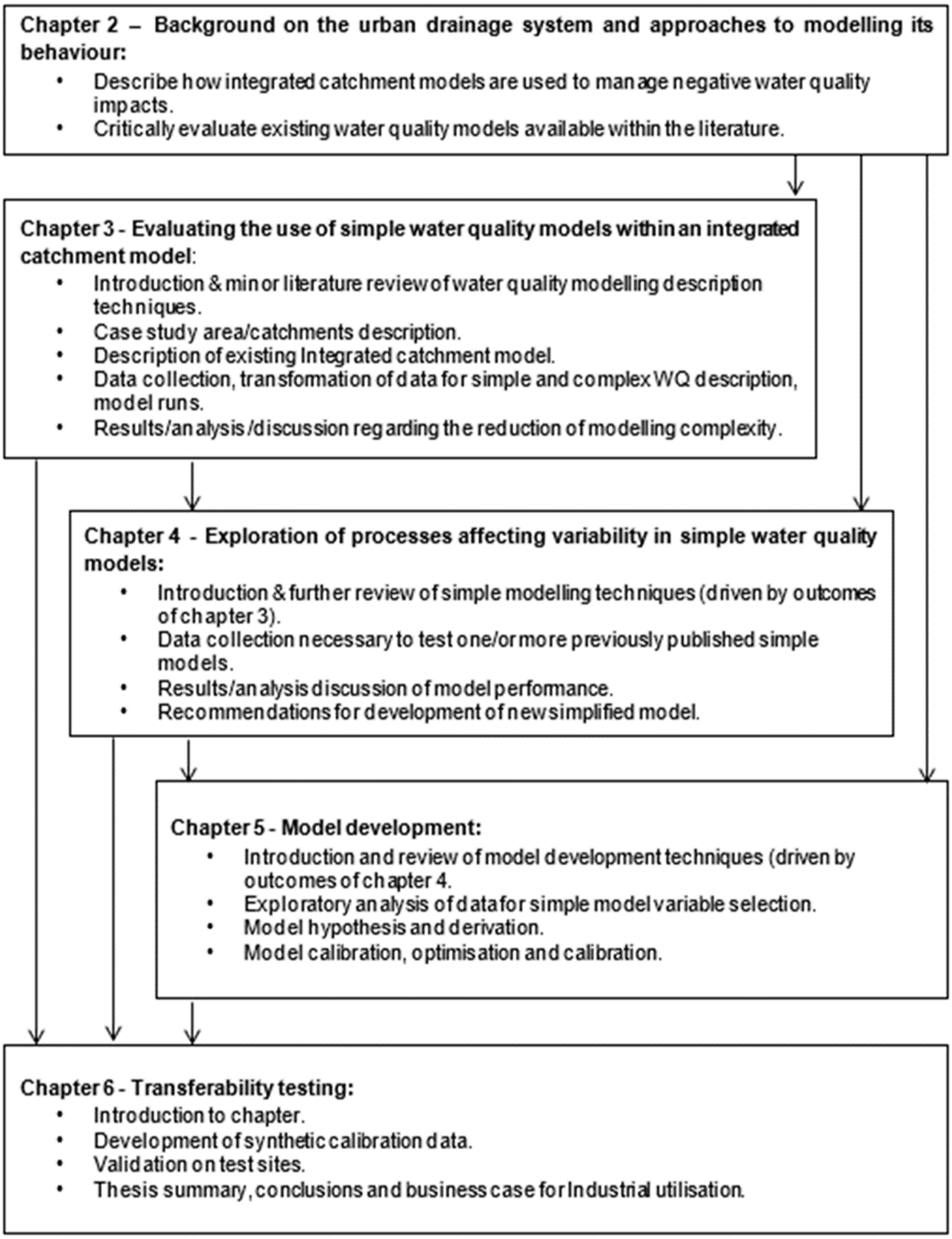

Figure 1-1 Schematic outline of research activities and their description

Information on the urban drainage system and the approaches used to model it has been presented in Chapter 2. Due to the broad aims of the research, and the issue that each chapter's direction is very much dependent on the outcomes of its predecessor, the scope of chapter 2 is limited to providing a sound scientific knowledge base as to how and why water quality models are used to protect the environment from the negative water quality impacts of urbanisation. To provide insight into the potential use of simple water quality models, Chapter 3 compares the performance of using water quality description techniques at varying temporal scales within an integrated catchment model. The chapter utilises a case study site, in that the integrated model has previously and is currently used by the water network and sewerage provider responsible for the management of urban drainage systems in the North-West of the United Kingdom. Chapter 4 explores the development and previous use of simple water models through the review of literature and the testing of one model on case study data, subsequently; all information presented through chapters 1 – 4 has been used to provide recommendations for the development of a new water quality model in chapter 5. Chapter 5 describes the development of a novel water quality model, following this, a Monte Carlo based technique has been incorporated into the model to allow the magnitude of uncertainty associated with its predictions to be established. Chapter 6 involves the testing of the new model on data other than where it was previously developed, allowing for discussion regarding its transferability. Chapter 7 concludes the work by summarising the previous chapters.

Chapter 2. Background to urban drainage systems and approaches to modelling their behaviour

2.1 Introduction

The purpose of this chapter, following the objectives of this thesis, is to present a solid foundation of science describing why and how water quality models are used to protect the aquatic environment from the negative impacts of urbanisation. Furthermore, a critical review of existing water quality modelling approaches has been presented, allowing for the research aims and objectives to be redefined, thus narrowing the scope of the research. This chapter is presented as follows:

- An introduction as to how and why urban drainage systems are used to manage the interaction between human activity and the natural water cycle.
- An overview of key water quality constituents and their respective impacts on receiving aquatic environments.
- An overview of the scientific processes which dictate water quality changes.
- A historical overview of the environmental legislation introduced to help guide UK water utilities manage the impacts of urban discharges. A detailed review of how the (UPM) Urban Pollution Management manual recommends solutions to manage the impacts or urban discharges should be conducted, as directed by the Water Framework Directive.
- A review of quantitative modelling techniques used to manage the impacts of urban discharges:

- An introduction into the concept of integrated catchment modelling; a process whereby quantitative models representing different parts of the urban drainage system (UDS) system are holistically integrated to simulate network water quality behaviour throughout catchments, ultimately aiding the design of schemes capable of protecting the water environment.
- A review of the problems associated with integrated water quality modelling and the need for new novel techniques which could improve its application.
- Chapter conclusions and redefinition of research aims.

2.2 The Urban Drainage System

Urban drainage systems are required to handle two types of water that occur from anthropogenic activity; wastewater and storm water. Water is important to every living organism; Humans extract it from the natural water cycle for sustenance, to meet the needs of industry and support general standards of living. Once used, it becomes adversely affected and is commonly referred to as ‘wastewater’. ‘Storm water’ is precipitation which has fallen on a developed area; its removal is required to prevent flooding and other health risks.

Whilst typical concentrations of constituents contained within waste and storm waters vary from catchment to catchment, these waters contain a wide range of potentially harmful constituents such as bacteria, viruses, minerals, nutrients, metals, dissolved and undissolved chemicals (Metcalf & Eddy *et al.*, 2003). The urban drainage system provides collection and passage of both waste and storm waters to designated treatment systems where constituents can be removed and degraded before being returned to the environment, thus minimising their potential adverse effects on human life and the environment (Butler and Davies, 2011).

The UDS sewerage system can be conceptually simplified as a network of interconnected manholes, pipes and structures designed to convey storm and wastewaters to a wastewater treatment works (WWTW). There are two types of conventional sewage system; the separate system, in which storm water and wastewater flows are collected and conveyed by separate structures, and the combined system, in which wastewater and storm water are handled together. Whilst the proportions of each system vary significantly and across the world, approximately 70% of the UK's sewerage infrastructure is estimated to be combined thus both systems and the respective flows are considered in this chapter of the thesis (Butler and Davies, 2011).

2.3 Urban Drainage System Discharges

Combined sewerage systems operate under two conditions; dry and wet weather flow. In wet weather conditions, flows within the UDS are normally up to five times the average dry weather flow, thus it is not feasible to allow full wet weather hydraulic capacity along the full length of sewerage infrastructure. If flow becomes sufficiently high, to prevent flows backing up the UDS, hydraulic relief is provided through Combined Sewer Overflows (CSO's). These structures divert and discharge flows above a certain threshold into a natural water course, continuation flow is conveyed to the WWTW for treatment. In separate sewage systems, it is most common for all collected storm water to be directly discharged into a receiving water body. Discharges from both these systems can have a negative impact on receiving water bodies, whilst these receiving water bodies are subject to different classifications of discharge (Table 2-1). Intermittent discharges, particularly those from combined sewer overflow spills, remain the biggest contributor to poor water body health (Ellis and Marsalek, 1996).

Table 2-1 Characterisation of Urban Discharges

Discharge classification	Discharge description	Example Polluter	Condition during occurrence
Intermittent	The release of emissions into the environment that occurs with interruption. Arise in the form of a process effluent. Relatively simple to trace back to a single source.	• WwTW's Inlet overflow • Combined Sewer Overflow (CSO) • Storm Tank Overflow (STO) • Pumping Station Overflow (PSO)	▪ • Wet
Continuous	The release of emissions into the environment that occurs without interruption. Arise in the form of a process effluent. Relatively simple to trace back to a single source.	• WwTW's effluent • Industrial premises	▪ • Wet and Dry
Diffuse	Pollution arising from land-use activities (urban and rural) that is dispersed across a catchment, or sub-catchment and does not arise as a process effluent, municipal sewage effluent, or farm effluent discharge. Difficult to trace back to a single source.	• Sheet field run off • Soil seepage • Mine seepage	• Wet

As one of the most significant threats to the preservation and protection of water body health, intermittent discharges remain the focus of this study. The impacts of intermittent discharges can be broadly categorized into having three different negative effects on the health of a receiving water bodies; reductions in water quality, public health issues and a negative aesthetic influence (House *et al.*, 1993) (Figure 2-1).

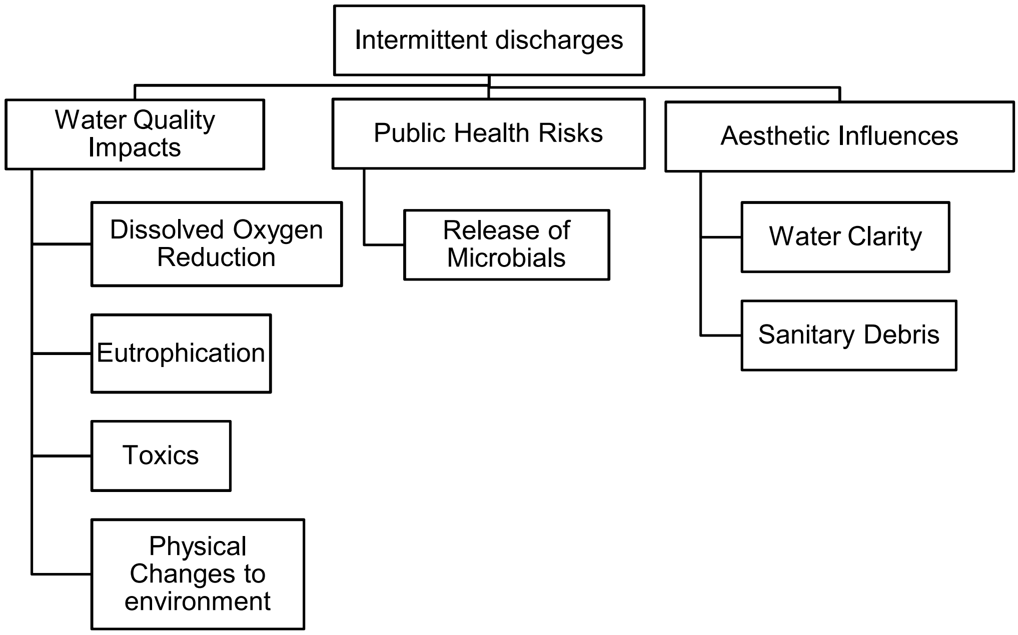

Figure 2-1 Negative Impacts associated with intermittent discharges

2.3 Water Quality

'Water quality' refers to the biological, physical and chemical characteristic of water. Whilst wastewater quality is variable with respect to location and time, it is typically comprised of organic and inorganic matter, and present in many forms; coarse grits to suspended solids, colloidal and soluble, these constituents are derived from; human excreta; undigested food wastes; washing and laundry products; industrial practises; the ingress of ground water into the sewerage system.

Stormwater quality varies further still, influenced by many different processes; it contains similar organic and inorganic matter to that of wastewater, with the addition of man-made substances derived from commercial, industrial practises and transport (House *et al.*, 1993). The major sources of matter contained within storm water are derived from: vehicle emissions; infrastructure corrosion and abrasion (mainly buildings and roads); bird and animal excreta; litter; green wastes (fallen leaves and grass residues) and chemical spills (House *et al.*, 1993).

2.3.1 Key water quality constituents

When evaluating the impact of urban discharges on receiving water body health, it is not practical to experimentally quantify the wide range of constituents pertaining to water quality, instead, several key pollutant indicators are used; Dissolved Oxygen Concentration (DO); Biological Oxygen demand (BOD); Chemical Oxygen Demand (COD); Ammonium (NH_4) and TSS (Total suspended solids).

With higher aquatic life forms requiring well oxygenated environments to thrive and a strong correlation existing between biodiversity and oxygen concentrations within aquatic environments; DO is the most critical and widely adopted indicator of water body 'health' (Makepeace, Smith and Stanley, 1995). Oxygen concentrations within receiving water bodies become depressed when mixed with urban discharges due to many different chemical and metabolic microbiological processes. Due to natural degradation processes, all receiving water bodies can 'self-purify', this occurs through re-oxygenation of the water body, whereby oxygen concentrations return to levels safe to the flora and fauna living within and around them. This ability, coupled with the varying levels at which water quality constituents become toxic to different flora and fauna, mean that to a certain extent, stormwater and wastewater discharges can be assimilated safely under certain constituent loading thresholds. However, if a water bodies assimilation capacity has been exceeded, constituents can cause a wide range of negative bio- chemical and physical impacts (Table 2-2).

Table 2-2 Negative impacts associated with exceedance of water quality thresholds within receiving water bodies – adapted from (House et al., 1993; Makepeace, Smith and Stanley, 1995; Ellis and Hvitved-Jacobsen, 1996).

Type of Impact	Water Quality Category	Water Quality Constituent	Effect of constituent on receiving waters
Biochemical and microbiological	Organic Compounds	• Carbohydrate; • Fats • Proteins	▪ • Depressed Oxygen levels

Type of Impact	Water Quality Category	Water Quality Constituent	Effect of constituent on receiving waters
	Solids	• Gross • Suspended • Volatile • Grit	• Increased turbidity • Reduced light penetration • Bed blanketing • Negative Impacts on mixing in rivers and lakes
	Nutrients	• Phosphorus • Nitrogen	• Eutrophication • Algal Blooming • Water discolouration • Odours • Depressed Oxygen Levels
	Hydrocarbons	• Aliphatic; • Aromatic; • Branch Chained; • Alicyclic;	• Development of surface water sheens; • Inhibition of atmospheric re-aeration • Depressed Oxygen Levels • Bioaccumulation of toxicants within aquatic species • Reduced ability for aquatic species to reproduce • Acutely toxic to aquatic species
	• Heavy Metal's • Pesticides	• Metalloids (particularly Arsenic); • Post Transition Metals (Copper, Zinc, Lead) • Organo-Chlorides	• Bioaccumulation of toxicants within aquatic species • Acutely toxic to aquatic species

Type of Impact	Water Quality Category	Water Quality Constituent	Effect of constituent on receiving waters
	FOG's (Complex Organic Molecules)	• Tri-glycerides • Di-glycerides, • Mono-glycerides	• Development of surface water sheens inhibiting oxygen transfer and atmospheric re-aeration
	Micro-Organisms and Viruses	• Faecal Coliforms, • Fecal Streptococci • E.coli, • Viruses (particularly enteric).	• Direct threat to the health of organisms (responsible for gastrointestinal disease in humans) • Groundwater Contamination
	Sulpherous Compounds	• Organic Sulphates	• Changes in water density altering mixing patterns; causing extension of low oxygen zones • Acutely toxic to aquatic species
Physical	Thermal effects	• Temperature changes	• Reduction of cold water habitat • Degradation of Fish health through disease resistance, growth and morality.
	Flow and Channel alteration	• Sediment erosion • Sediment deposition • Mixing	• Degraded habitats due to channelization • Decline in species biological integrity

Type of Impact	Water Quality Category	Water Quality Constituent	Effect of constituent on receiving waters
	Flow and Channel alteration		

Chemical oxygen demand (COD) is used to give an indirect indication of the total amount of organic matter present in water; Biological oxygen demand (BOD) gives an indirect indication as to what fraction of organic matter is readily biodegradable. Solids are also regarded as an important indicator of urban pollution, as efficient carriers of pollutants, the fine fraction of TSS is specifically associated with problematic pollutants such as metals and attached nutrients (Sartor, Boyd and Agardy, 1974; Deletic, Maksimovic and Ivetic, 1997). Typical concentration values of key water quality indicators are presented in Table 2-3, they are expressed in terms of their range and event mean concentration (EMC); the EMC is a representative value of the average pollutant concentration.

Table 2-3 Concentration ranges and event mean concentrations for key water quality indicators.

WQ Parameter	Wastewater			Stormwater		
	Ainger et al.,(1997)		Metcalf and Eddy (1977)	U.S. EPA (1983)	Ellis and Mitchel (2006)	
	Range (mg/l)	EMC (mg/l)	Range (mg/)	Range (mg/l)	Range (mg/l)	EMC (mg/l)
TSS	180 - 450	300	270 - 550	67 - 101	21 – 2582	190
BOD	200 - 400	300	60 - 220	8 - 10	7 – 22	11
COD	350 - 750	550	260 - 480	40 - 73	20 – 365	85
NH_4	30 - 85	60	4 - 17	0.43 - 1	0.4 - 20	1.45
P	15	-	1.2 - 2.8	0.67 - 1.66	0.02 - 4.3	0.34

Typical values of key water quality indicators recorded at spilling CSO's situated within combined drainage systems are presented in Table 2-4, in this case, the EMC is a representative value of the average pollutant concentration of the spilling discharge.

Table 2-4 Key Water Quality Indicator concentrations recorded from CSO spills in combined systems referenced within the literature.

Water Quality Parameter	EMC (mg/l)	EMC (mg/l)	Range (mg/l)	Range (mg/l)
	Ellis (1996)	Lager et al., (1997)	NWRW (1991)	Suarez and Puertas (2005)
TSS	425	370	105 - 320	421 - 733

BOD	90	115	40 – 124	166 - 389
COD	380	367	148 - 389	293 - 834

2.4 Management of Urban Discharges

Water utilities seek to reduce the impacts of urban discharges on receiving water bodies by investing resource into new and existing solutions; these solutions are based upon the respective utilities understanding of the water cycle and how the individual components of catchments under their jurisdiction interact within it. This understanding is fundamentally provided by simulating the water system via the use of quantitative modelling techniques. It is therefore of significant benefit to UK water companies and to the wider public that the modelling techniques and methodologies deployed within utilities incorporate the latest and most effective science to ensure the realization of efficient solutions that meet the challenges of the present and future. This is of particularly note because many previously designed solutions to urban drainage issue will have been designed in the last 50 years, thus investment decisions made in the present will have implications well into the future when conditions under which these solutions operate may be subject to change, hence why future scenario analysis is an important and useful concept within urban drainage modelling (Niemczynowicz, 1999; Butler and Davies, 2011).

Conventional practice in the UK water Industry has been to manage and, therefore, model the various components of the engineered urban wastewater cycle (urban drainage, WWTW and receiving water body) in isolation (Butler and Davies, 2011). Each component has been engineered to meet the needs of its users and the environment, but with little feedback or cross-reference to other components. This approach led to increasing pressure to investigate the relationships between individual components of the cycle (Butler and Davies, 2011). In 1994, Following the development of a major research program funded by the entire UK water industry, the Urban Pollution Management Manual (UPM) was released as a method of guidance to the management of pollutant discharges (UPM. FWR. 1st edition (1994); UPM. 2nd edition. (1998); UPM. 3rd edition. (2012). There are three recurring themes in the guidance:

- Analysis should be holistic, covering all elements in the sewer system itself, the wastewater treatment works and receiving river.
- The level of detail of any study, and in particular; the models used, should be appropriate and that, in the right circumstances, a holistic approach may also be simple.
- The approach should be underpinned by relevant environmental standards with models able to demonstrate compliance with those standards.

Many of the planning concepts and enabling tools in the manual were substantially new at that time and addressed issues that were, and continue to be, of great importance to the industry, the intervening period has seen widespread adoption and application of the procedure throughout the UK and in the areas having acute combined sewer overflow problems. To fully understand the terminology and direction given with the UPM, the concept of water quality model classification must first be discussed.

For any receiving water impact study, regardless of whether the system being modelled is combined or separate, quantification of the water quality constituents present within wastewater and storm water flows is necessary to provide information to a receiving water impact model. Water quality models provide this information by describing water quality constituents (pollutants) entering, travelling through and (most importantly) leaving the sewer or storm water system.

Pollutants are derived from two major sources; the catchment surface and wastewater. Predicting generation of pollutants in the form of wastewaters is relatively simple as base flows of pollutants into the sewer system tend to follow a regular diurnal profile ((Metcalf & Eddy *et al.*, 2003)). Storm water pollutant generation is stochastic in nature, pollutant 'build-up' is the overarching term used to encompass the different processes which contribute to the generation of pollutants on the catchment surface during dry weather, 'wash-off' is the overarching term used to describe the many different processes whereby accumulated pollutants become mobilized during storm water runoff events. Different catchment and event characteristics have been cited as influential on build-up and wash-off processes (Table 2-5) (Brodie and Rosewell, 2007;

Goonetilleke, Egodawatta and Kitchen, 2009; Murphy, Cochrane and O'Sullivan, 2015).

Table 2-5 Catchment characteristic influencing variations in storm water quality entering the urban drainage system.

Build-Up	Wash-off
Land use	Rainfall characteristics
Population	Topography
Traffic flow	Solids characteristics
Street cleaning	Street surface conditions
Season of year	
Meteorological conditions	
Antecedent dry weather period	
Street surface condition	

Once within the sewer system, pollutants are subjected to a number of different in-sewer processes; hydrodynamics, mixing, advection-dispersion, biotransformation, sedimentation/resuspension, sediment erosion and deposition (Ashley, Hvitved-Jacobsen and Bertrand-Krajewski, 1999; Butler and Davies, 2011).

The pollutants can pass through to the receiving water body untransformed or become deposited; these deposited pollutants can then be subsequently re-eroded at a later date (commonly during a rainfall event), causing significant variation to the original water quality characteristics of wastewater and stormwater (Ellis and Marsalek, 1996; Ashley, Hvitved-Jacobsen and Bertrand-Krajewski, 1999; Mannina *et al.*, 2012). Water quality models, are utilized to objectively quantify the concentrations of water quality constituents discharged into the receiving water body, however the quantitative methods and processes they use can vary significantly, a classification of available quantitative water quality techniques has therefore been provided.

2.4.5 Water Quality Models

In the context of urban drainage and water quality modelling, authors' have various definitions, descriptions and use a range of terminology to classify models, thus the classification of water quality models is an ambiguous process (Korving, 2004; Schellart, A. N. A., Tait, S. J., and Ashley, R. M. 2010). This section attempts to provide classification and provide a review of the types of water quality models within each classification. Examples of models currently used by practitioners and the research field have been provided and their methods of simulating water quality processes presented, hydraulic simulation processes have been largely ignored due to the scope of the thesis.

Korving (2004) presented the following classification system with respect to models used commonly used within the urban drainage field:

- Physically based or 'white-box' models. These models describe the fundamental physics and solve governing equations affecting water quality. These models will often attempt to describe complex processes such as advection-dispersion, sedimentation/resuspension and sediment transport behaviour within sewer and storm water systems. A strictly physical water quality models computational approach would involve the use of equations and relationships in which all in which all parameters were measurable physical quantities, however in practise, even the most physical of water quality models benefit from calibration due to the inherent empirical nature of certain scientific phenomena (Box, Jenkins and Reinsel, 1994).
- Conceptual or 'grey box' models. Conceptual use equations used are calibrated input-output relationships that simulate the functional behaviour of water quality processes under observation (Harremoës and Madsen, 1999).
- Statistical and Empirical, or 'black box' models. These models calibrate a statistical relationship between inputs and outputs, without attempt to describe the behaviour of water quality processes ((Harremoës and Madsen, 1999)).

Physically based or 'white-box' models

Harremoes and Madsen (1999) presented a similar modelling classification system, adding a further differentiation between stochastic and deterministic models. Harremoes and Madsen (1999) described stochastically based models as simple models often associated with expressing the accuracy of the system under observation, in the context of environmental modelling, stochastic models often utilise regression functions and transfer functions. It has been suggested that if any random variables with assigned probability distributions are used within a model, then the model is deemed stochastic, otherwise it can be classified as deterministic (Clark, 1973). In simplistic terms, deterministic models use a single set of input values and a single parameter set to generate a single set of outputs, thus they do not account for randomness with the same input values generating the same outputs values. Stochastic models represent some/or all of the inputs and parameter values as statistical distributions, for example, a standard deviation of a particular value i.e. catchment build-up capacity, can be applied to generate an array of output values, each derived from different combination of the inputs and parameters and/or each of them related to a certain probability of occurrence. These techniques are often utilised to quantify uncertainty/error associated with model inputs (Larson and Schubert, 1979). Unlike deterministic models, stochastic models commonly require the model to be run many times, each run with a different combination of parameters or model inputs, resulting in many outputs that can be analysed to define probability distributions of model outputs. Whilst it is widely accepted that no model can be fully deterministic due to the probability that not all physical phenomenon can be mathematically described and exactly calculated, these models attempt to deterministically simulate the key processes involved in determining water quality (Box, Jenkins and Reinsel, 1994).

With respect to urban drainage water quality modelling, various deterministic water quality models are available to researchers and practitioners such as the United States Environmental Protection Agencies Storm Water Management Model (SWMM) (us-epa, www.epa.gov), the Danish Hydraulic Institute for Water and Environment (DHI) (www.dhi.dk/mouse) MOUSE and the Wallingford Software package InfoWorks CS (www.wallingfordsoftware.co.uk).

SWMM is a distributed discrete time simulation model. SWMMs surface build-up module utilises Sartor and Boyd's (1972) nonlinear function of dry days to estimate pollutant build up for different land uses on the catchment surface; different functional options (power, exponential and saturation) are available within the model. For pollutant wash-off, SWMM offers a more simplified method of calculation. Research by Ammon (1979) concluded that whilst sediment transport theories are attractive to users, field data requirements to derive parameters involved in sediment transport theory are significantly large, SWMM therefore offers different empirical models to represent wash-off of pollutants from the catchment surface; exponential wash-off, rating curve wash-off and EMC wash-off. For pollutant transport, SWMM offers numerical solution of the 1-D Advection-dispersion equation , the model further assumes complete mixing within conduits via the form of a continuously stirred tank reactor model (Rossman, 2010).

DHI Water & Environment developed the model MOUSE, it contains several modules capable of modelling pollutant processes, these modules are collectively known as MOUSETRAP. MOUSETRAP utilises a surface runoff quality module capable of simulating the build-up and wash-off of pollutants, a sediment transport module with the option of four different transport equations, an advection-dispersion module to compute pollutants advection and dispersion through the drainage network and a water quality process module to compute processes such as re-aeration, oxygen consumption from BOD/COD, biofilm and erosion of sediment and growth of suspension biomass (Bouteligier, Vaes and Berlamont, 2002).

InfoWorks CS is a later version and update of the software Hydroworks, which was developed by merging previous models FLUPOL and MOSQITO (Ashley, Hvitved-Jacobsen and Bertrand-Krajewski, 1999). InfoWorks CS includes modules for pollutant surface build-up and wash-off, erosion and deposition, gully-pot build up and a variety of different solids transport modules; this will be discussed in greater detail within this thesis.

'Conceptual or 'grey box' models

Whilst often not strictly conceptual in their methods of calculation, examples of 'grey box' models examples of commonly utilised conceptual models within urban drainage studies are Monash Universities Urban Stormwater Improvement Conceptualisation Model (MUSIC) (https://toolkit.ewater.org.au /Tools/MUSIC/ features) and the Leibniz Institute for Freshwater Ecology and Inland Fisheries Nutrient Emissions in River Systems Model MONERIS (http://moneris,igb-berlin.de) These types of models commonly conceptualise pollutant processes in urban catchments (Bach *et al.*, 2014).

MUSIC allows conceptualisation of stormwater management systems such that urban catchment management measures can be evaluated in an integrated manner. MUSIC can be used to model various types of pollutant generated from urban areas using a stochastic process involving cross correlation between total suspended solids and other pollutants; and serial correlations of water quality time series. MUSIC's pollutant generation process is based on statistical analysis or urban stormwater pollutants by Duncan (1999) and utilises a conceptual rainfall-runoff model developed by (Chiew at al., 1997), furthermore, conceptualised parcels of water carrying pollutants are assumed to exponentially decay towards an equilibrium value through strings of continuously stirred tank reactors (CSTRs), this behaviour is described in the model by first-order decay kinetics (Chiew *et al.*, 1997; Duncan, 1999).

MONERIS (Modelling Nutrient Emissions in River Systems) is a semi-empirical, conceptual model for the quantification of nutrient emissions from point and diffuse sources in river catchments (Behrendt *et al.*, 2003). The MONERIS model contains eight sub modules to simulate the main processes involved in the generation of pollutants and the transport of suspended solids and nutrients into a river network. The MONERIS model utilises a geographical information system (GIS) to support environmental impact studies in a watershed-based approach. Complex pollutant generation and transport processes are simplified using a GIS based model with empirical characteristics. The conceptual approach can be used to quantify nutrient emissions from non-point and point sources in river catchments larger than 50 km^2 (Huber *et al.*, 1999). The key processes and pathways modelled in MONERIS are groundwater, erosion, overland flow, drainage, deposition of atmospheric pollutants on water surface areas, urban areas and point sources (e.g. wastewater treatment plants) (Huber *et al.*, 1999).

Statistical and Empirical, or ‘black box’ models

Black box models are those that solely calibrate a statistical relationship between inputs and outputs, without any attempt to describe physical water quality processes. Parameters utilised within these models are statically derived through regression techniques to determine the relationship between the model input and model output. Statistical end empirical models utilised within the urban water quality modelling field commonly use regression equations to estimate event-based water quality loads. They focus on relating measurable quantities with measurable physical parameters considered key to the process under observation such as rainfall intensity and catchment parameters such as impervious area, land-use and catchment slope (Vaze and Chiew, 2003). Stochastic approaches are regularly employed within these types of models. There are many examples within the literature where empirically functions have been derived to predict water quality event loads by relation to stormwater characteristics (Driver and Tasker, 1988; Driver and Troutman, 1989; Maniquiz, Lee and Kim, 2010). Examples of process based empirical water quality models that attempt to simulate processes such as pollutant build-up and wash-off from the catchment surface include (Geiger & Dorsch, 1980; Hemain, 1986; Huber and Dickinson 1980; Jewell & Adrian, 1982). These models are often limited in that the statistical relationships they derive are limited to the given set of data which represents on spatial arrangement. They are often employed for planning purposes only or in cases where insufficient data is available to develop a more detailed representation of the processes under observation (Elliott and Trowsdale, 2007).

The way, in which water quality models utilize input data, the number of processes (if any at all) and the amount of data available for calibration ultimately affects model predictive performance. Figure 2-2 shows the relationship between model complexity, data availability and consequent predictive performance (Grayson and Bloschl, 2000).

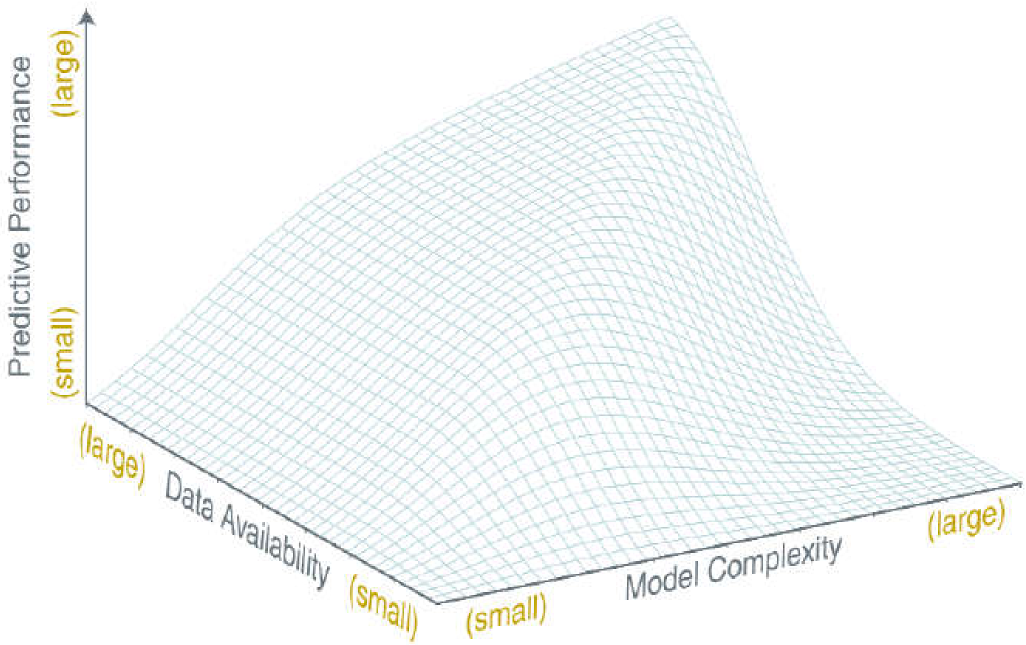

Figure 2-2 Visual interpretation of model characteristic relationships – (Grayson and Bloschl, 2000)

2.5 Legislation

In the year 2000, the European Union (EU) adopted the Water Framework Directive (WFD) (2000/60/EC). It is a legislative method to managing and protecting water, constructed not on national or political boundaries but on natural hydrological and geographical formations: river basins. It requires coordination of several EU policies, and prescribes a scheduled timetable for action, 2015 was the targeted date for transforming European waters into 'good' condition (Kallis and Butler, 2001), the WFD required that European countries produces river basin management plans to achieved this 'good' status. The aim of the procedures defined within it are focussed on combating the deterioration of water resources in the member state territories. Water quality models play a significant role in meeting the aims of the WFD, through providing a means of assessment of water quality, directing trends of water quality parameters and through identification of alternative actions and measures identified within each member states river basin management plans. The assessment of water bodies proved to be a difficult goal, linked to sufficient lack of data associated with river basins and the absence of systematic measures regarding the involved parameters associated with water quality (Tsakiris and Alexakis, 2012).

Annex V of the WFD (European Commision, 2000) provides standard definitions for the classification of water bodies into five ecological quality classes: high, good, moderate, poor and bad. The requirements for the good, moderate and high classifications are presented as follows:

- High status – No or very minor deviation from an undisturbed (reference) condition.
- Moderate status – Moderate deviation from the reference condition.
- Good status – Slight deviation from reference condition.

With respect to the WFDs reference assessment process, water quality parameters for a given surface water body is expressed as ecological quality ratios (EQR). EQR's consist of the observed parameter in the water body divided by the same parameter in the reference condition.

The EU Water Framework Directive (WFD) specifies a sophisticated and holistic assessment of the water quality within a catchment in order to meet environmental and ecological objectives, specifically, it requires a "combined approach" of emission limit values and quality standards (Borja *et al.*, 2004). With the key guiding goal is to achieve 'good status' of ground and surface waters; 'good' meaning that water bodies meet the standards established in the existing member stated water directives and in addition new ecological and emission standards. In the UK, water quality standards designed to protect aquatic life from urban discharges are the Fundamental Intermittent standards and percentile standards (FWR, 2012). Percentile standards are standards that are failed if the concentration of a pollutant is greater than the standards for 1% or more of the time; they are designed to help manage the risk posed by continuous discharges. Fundamental Intermittent standards (FIS) are expressed in terms of DO and un-ionised ammonia, these two determinand's have the most direct impact upon the health of fish and invertebrates, the standards are expressed in terms of concentration-duration thresholds and allowable return period or frequency, simply, predetermined concentration duration thresholds (CDT)s for DO and un-ionised ammonia must not be breached more frequently than shown in Table 2-6 (for salmonid and cyprinid fisheries) Table 2-7. They are designed to help manage the risk posed specifically by intermittent discharges.

Table 2-6 Fundamental Intermittent Standards for DO – concentration/duration thresholds not to be breached more frequently than shown (values are appropriate for salmonid and cyprinical fisheries).

	Receiving river DO concentrations (mg/l)		
Return Period	1 hour	6 hours	24 hours
1 month	4.0	5.0	5.5
3 months	3.5	4.5	5.0
1 year	3.0	4.0	4.5

Table 2-7 Fundamental Intermittent Standards for Un-ionised ammonia - concentration/duration thresholds not to be breached more frequently than shown (values are appropriate for salmonid and cyprinical fisheries).

	Receiving river DO concentrations (mg/l)		
Return Period	1 hour	6 hours	24 hours
1 month	0.150	0.075	0.030
3 months	0.225	0.125	0.050
1 year	0.250	0.150	0.065

FIS standards can be impractical to work with directly as considerable knowledge concerning the transport and reaction of pollutants after a discharge event and the in-river chemistry is needed. Because this knowledge is sometimes inaccessible privy to the use of field surveys and river modelling, 'derived' standards based on BOD and total ammonia have been developed. The standards are focused at the point of mixing and thus require no knowledge concerning following transport or degradation processes. It is difficult to present these 'derived' thus they are not described in this thesis, further information on all receiving water quality standards can be found within the Urban Pollution Management manual (FWR 2012).

The WFD requires a management plan for each river basin to be developed every 6 years. In England and Wales, the Environment Agency are the competent authority for carrying out the objectives of the WFD achieved by assessing receiving waters against the WFD standards and in respect of managing the negative impacts on aquatic life within the UK: existing FIS and 99 percentile standards (DoE, 1977). With the implementation of the Water Framework Directive (2000/60/EC) (WFD) and its new water quality and ecological standards, the FIS and 99 percentiles standards have been reviewed (Environment Agency, 2012). The work compared the UPM FIS with WFD emission standards and indicated that the UPM FIS were “fit for purpose” and that for concentration/duration/frequency combinations the UPM standards for dissolved oxygen and ammonia provided a margin of safety for salmonid and cyprinid fisheries and that meeting UPM FIS standards would ensure that ‘good’ quality status of UK water bodies would be maintained. With regard to UPM 99% standards, the report indicated that they should continue to protect freshwater aquatic life from intermittent urban wet weather discharges and ensure that the existing ‘good’ quality status of a water body is not compromised. The report does however recommended that the WFD emission standards should be presented to the United Kingdom Technical Advisory Group to confirm suitability within the WFD and that UPM FIS and percentile standards be modified into a revised version of the UPM, however, in the intervening period, standards should continue to be used by regulators in preparing permit applications and in designing solutions to urban discharges (Environment Agency, 2012).

Whilst the EA highlight and provide the need for investigation into failing watercourses, it is the responsibility of the respective wastewater service provider under whose jurisdiction the water body falls to provide a means of managing the impacts of pollution. To meet this responsibility, UK water companies endeavour to objectively evaluate the impacts of pollution on water receiving water bodies, this is done by simulating the behaviour and of the urban water system; information which is provided by numerical hydraulic and water quality modelling studies.

Water quality modelling studies allow practitioners to assess the compliance of their river systems against water quality standards and to identify, with supporting information on existing river condition, potential locations where discharges may be contributing to failing watercourses. Moreover, the studies enable UK water companies to design rehabilitation schemes and structures to remediate any failing watercourse and further justify the capital investment needed to finance them to the Water Industries economic regulator OFWAT, thus satisfying the needs of the EA and protecting the health of the aquatic environment (Butler & Davis, 2010).

2.6.1 Urban Pollution Management Manual

The UPM procedure recommends four main phases for the management of urban pollution:

- Initial Planning.
- Assembling Data and Tools.
- Developing Solutions.
- Consenting and Detailed Design.

A review of each of these stages is presented.

2.6.1.1 Part A – Initial Planning

Part A of the methodology is concerned providing an Initial assessment about the nature and severity of the pollution problem. The methodology can be separated into three distinct components;

  - Preliminary assessment of wet weather problems.
  - Framework for environmental assessment
  - Initial choice of data and tools needed.
  - Preliminary Assessment of Wet Weather Problems

This section of the methodology provides guidance concerning the steps which should be taken for identification and severity assessment of wet weather discharges on local watercourses and coastal waters. The identification of 'satisfactory', 'unsatisfactory' and 'very unsatisfactory' is advised through utilization of a CSO impact methodology Milne *et al*., (1992) according to NRA, (1995). Furthermore, an assessment of storm tank overflows and coastal impacts is also recommended; concluding with judgement on overall UPM study needs.

Framework for environmental assessment

The aim of this section of the methodology is to establish an overall environmental framework for the planning study. Establishment of receiving water standards to be used throughout the study is first addressed. The desired Environmental Quality Objectives (EQOs) are defined as well as the Environmental Quality Standards (EQSs) necessary to provide reference against which the quality of a water body can be judged; and whether any future solution will provide adequate environmental protection (DoE, 1977).

Intermittent discharges can impact surface waters with a variety of uses; river aquatic life, bathing and general amenity (Crabtree *et al.*, 1994). Due to the scope of this thesis, presentation of the UPM procedure is with respect to the management of urban discharges on river aquatic life.

Initial choice of data and tools needed

This stage of the UPM methodology is concerned with the data and tools required and to be developed based on relative importance of different discharges and the complexity of water quality interactions. The manual recommends selection of the simplest tools that are likely to be required, consistent with generating a safe solution; and that technical complexity and cost are important factors that should be reflected in the selection of the final data and tools. The development of tools to simulate discharges to rivers is necessary, this process can be separated into the need to simulate the following components for discharges to rivers (adapted from FWR, 2012);

- Rainfall Inputs, choice between:
    - Design storms - recommended for catchments up to about 5,000 population;
    - Long rainfall time series – give better interaction between rainfall and, for example, river flows and the build-up of pollutants during dry periods.
- Upstream river flows and quality, choice between:
    - River flow/quality frequency distributions; or,
    - Daily rainfall/river flows.
- Sewer flows, choice between:

        - A simple tank simulation model; or,
        - A detailed sewer flow model - usually necessary when the sewer system is hydraulically complex with numerous CSO's, such that spill volumes and frequencies cannot be adequately asses using a simple tank model.
    - Sewer quality, choice between using;
        - Simple methods for estimating BOD and ammonia concentrations; or,
        - Detailed quality simulation models, usually required if:
            - The sewer system is large, complex and flat such that detailed knowledge about sewer sediments (quantities, characteristics and behavior) is needed; and/or,
        - Sewage treatment effluent is a major factor affecting in river quality.
    - Sewage treatment effluent, choice between;
        - Effluent flows and quality distributions; and/or,
        - A detailed STW quality model.
    - The impact of discharges in rivers, choice between using:
        - Simple mass balance with the derived intermittent standards; or,
        - Detailed driver impact model to derived equivalent standards on a site-specific basis and simple mass balance to check compliance with standards.

2.6.1.2 Part B - Assembling Data and Tools

The second phase of the UPM procedure involves assembling key data such that the appropriate tools (identified in Part A) can be used for the study. This part of the UPM procedure has an increased focus on the tools and approaches available to perform the simulations specified in the Initial choice of data and tools needed section.

Rainfall Modelling

Rainfall is a key driver when considering the wet weather performance of urban drainage systems; its representation as an input to simulation models is crucial to an understanding of the drainage system under analysis and subsequently the development of solutions. The various options for the development of rainfall inputs is discussed in this section.

Synthetic Design Storms

Research into UK Floods by the NERC (1975) led to the development of the Wallingford Procedure design storms. The storms (a series of synthetic design storms) were developed specifically to be suitable for hydraulic design and the analysis of sewer systems. The design storm is an idealized storm profile to which a statistically-based return period has been attached, its time pattern is deigned to mimic the 'shape' of an observed storm, They allow urban drainage practitioners to construct rainfall time timeseries of any depth, return period and duration (greater than one year) allowing for the most severe response of the urban drainage system to be examined.

Annual Time Series Rainfall

To account for rainfall characteristic across different regions within the UK, (Henderson, 1986) developed Annual Time Series Rainfall (TSR), these are a number of series of real storms, each representing a typical year for different regions in the UK. These storms are typically used to investigate the hydraulic performance of existing systems but are limited in that the regionalization procedure is crude, extreme events are not included and return periods cannot be assigned to events; thus, checking for compliance with intermittent river standards cannot be performed.

Long Rainfall Time Series

The limitations of using Synthetic Design Storms and Annual Time Series Rainfall stem from the issues associated with their development; original rainfall data has been filtered to create a simplified set of storms, thus the application of these storms can be limited to certain types of analysis. Working with long rainfall time series can overcome these problems. Work by the Water Research Council (WRC) led to the design of the rainfall processing package (STORMPAC) (WRC, 1994). The package gives practitioners an alternative solution by providing modules which allow for:

- Synthesizing long time series of hourly rainfall for any location in the UK.

- Identification of storm events from either synthetic of historical series.
- The ability to select storm events based on characteristics specified by the user.

STORMPAC contains a stochastic rainfall generator (SRG) which by specifying a grid reference, altitude, the distance from the coast and mean daily rainfall for each month allows practitioners to obtain long term localised long term rainfall series data representative of an area (Henderson, 1986). An alternative to using SRG data is the use of historical rainfall time series data, these hourly rainfall data sets can be obtained from the Meteorological office.

Following consideration of the available rainfall data and the purpose of the UPM study, practitioners are required to select 'events' suitable for the study. In respect of protecting river aquatic life, the events recommended for selection are all events which could cause failure to meet the one-year return period threshold for BOD and Ammonia.

2.6.2.2 Upstream River Flow and Quality

This section describes the alternative approaches available for generating upstream river flows and qualities to be used as boundary conditions within river impact modelling.

River flows and quality conditions at the time of a storm are influenced by many factors:

- The size, land use and geology of a catchment.
- The time of year.
- Rainfall patterns over previous days.
- Upstream discharges and abstractions.

Statistical procedures whereby repeated mass balance calculations during which the estimated storm induced urban discharges are mixed with river flows selected from appropriate frequency distributions are recommended.

River flow frequency distributions are usually expressed by flow duration curves which give the daily mean flows which are exceeded for different proportions of time. Summer flows are critical for intermittent pollution events as low flow conditions and high temperatures reduce dissolved oxygen levels within rivers and increase the potential for high concentrations of un-ionized ammonia due to reduced dilution effects.

Hydrological models can be used to estimate river flow frequency distributions, these rainfall-runoff model create time series of daily mean flows based on long rainfall time series and evaporation data. Several models are available to perform this task, they often use simplified representations of the main physical processes (interception, evapotranspiration, transfers between soil, groundwater and channel storages and times of travel) governing water flow in a river catchment.

The use of existing river quality data is necessary for estimating upstream river quality distributions for BOD and ammonia. An example of upstream river condition data is presented in table 2-8.

Time (s)	NH_4 (mg/l)
0	0.0410692
3600	0.0462924
7200	0.0328054
10800	0.0224986
14400	0.0301561
18000	0.039995
21600	0.457389
25200	0.617807
28800	0.454406
32400	0.313387
36000	0.160158
39600	0.0622826
43200	0.0349556
46800	0.0276046
50400	0.0383101
54000	0.0273219

Table 2-8 Upstream NH_4 river concentration data collected May 2003 from an independent dye tracing experiment conducted in The Chillan River.

The accuracy of upstream river flow quality is less important than the estimation of river flows or discharge quantities because in-river concentrations which are allowed for short durations are generally much higher than background river concentrations (FWR, 2012).

2.6.2.3 Sewer Flow Modelling

Hydraulic understanding of a sewer system is necessary to perform a pollution assessment study, to make realistic predictions of temporal variations in pollutant concentrations and loads it is essential to understand how flows vary during and before storm events.

Various detailed sewer flow models at very levels of detail are available to practitioners. For most pollutions studies a detailed flow sewer model will be necessary however the level of detail can be varied depending on the requirements of the study. Specified rainfall profiles are routed through the modelled pipe network to produce surface runoff hydrographs, depths and flows are estimated throughout the sewer network at each timestep allowing surcharge and flooding at manholes to be predicted. Model simulation performance should be checked (model verification) using historical data and against specific field measurements. The models should account for all flows and loads that are discharged into the river or rivers under analysis (WRC, 1993; FWR, 2012).

If dynamic sewer modelling is required, a high level of accuracy over a wider range of flows is required to estimate the erosion and depositions of sewer sediments (a major pollutant source). In situations where there is little interaction between CSOs because of relatively small catchments and where the continuation flow can be estimated with significant confidence, it is considered reasonable in the procedure to estimate spill volumes via simple tank models (WRC, 1993; FWR, 2012).

Sewer Quality Modelling

This section introduces the processes which affect pollutant loads during wet periods. The ability to model these processes is discusses and a brief introduction to the sewer quality models (SQMs) presented.

Pollutant loads carried by and discharged from sewer systems vary in a complex way as many different processes are involved. Dry weather processes contribute to the build-up of sediments on the catchment surface forming an important source of pollutants when later mobilized by rainfall and higher flows that occur during wet weather (Ball, Jenks and Aubourg, 1998). The key processes influencing the variability of pollutant loads are (Crabtree, 1989; Bouteligier, Vaes and Berlamont, 2002; Kanso, Chebbo and Tassin, 2005; Obropta and Kardos, 2007b):

- Foul Inputs.
- Build-up and wash-off of sediments from the catchment surface.
- Deposition and erosion of sediments within the sewer system.
- In sewer sediment transport.
- Advection and dispersion of pollutants.
- Biochemical reactions.

Domestic, commercial and industrial effluents all enter the sewer system as ‘foul’ inputs. These inputs will vary spatially and temporally from catchment to catchment, they are typically affected by a diurnal profile. During storm events, sediments and attached pollutants are washed from surfaces and enter the sewer system. The quantities of these sediments are linked to the intensity of rainfall and the quantity/availability of these sediments to be washed-off from the catchment surface (Bai and Li, 2013). When flow velocities are low in the sewer system, suspended sediments can settle out of the flow and deposit on the sewer bed. This process is influenced by:

- Size of sediment particles.
- Density of sediment particles.
- The flow regime.

Sediments that make it into the sewer system flow, they move down the system as bed load or in suspension. Deposited sediments can act as a store of pollutants within the sewer system. As flow rates increase, deposited sediments can be eroded again back into the flow, this phenomenon is influenced by: (Schellart, 2007):

- The flow velocity.

- The width of sediment bed.
- Characteristics of the sediment bed.
- The shear strength of the sediment bed.

The processes of advection and dispersion govern the way pollutants travel down the sewer system, the former – advection - is the main pollutant movement process. The total quantities of pollutants in the sewer system can change due to biochemical reactions which occur in the sewer system. In terms of the pollutant load discharged during wet weather, the approaches available to model sewer system performance are broadly defined in the UPM manual as either being:

- Simple tank simulation models.
- Detailed flow sewer models and subsequently the use of event mean spill concentrations.
- Detailed dynamic sewer quality models.

Simple tank simulation models give practitioners the ability to model multiple events or long chronological rainfall sequences rapidly because flow processes are represented by tanks in series and in parallel. These tanks receive runoff and foul flows from different sub-catchments, pollutants in these models can be modelled in a variety of ways, for example, foul flows and runoff are assigned event mean concentrations allowing loads at any point in the system to be calculated via a mass balance procedure. Another method of modelling pollutants in simple tank simulation models is by representing sediment stores in the tanks, allowing erosion to occur at a constant concentration by runoff, this allows effects such as the 'first-flush' to be simulated (FWR, 2012).

Detailed dynamic sewer quality models are most commonly used in the delivery of the UPM procedure, a variety of detailed models are available to practitioners, examples are:

- Storm Water Management Model (SWMM) (US-EPA, www.epa.gov).
- MOUSTRAP (www.dhi.gk/mouse).
- INFOWORKS CS (www.Innovyze.com).

These types of models typically contain sub models which can be used to simulate:

- Foul inputs;
- Surface wash off;
- Pollutant and sediment behavior within pipes;
- Pollutant and sediment behavior within tanks.

Dynamic SQMs assign land uses to sub-catchment areas to estimate foul inputs from domestic sources; these are represented with diurnal variations in flow and quality. A variety of different approaches to surface wash-off are available within and between different SQMs, ranging from the simple - sediment sources are eroded at a rate that is proportional to rainfall intensity – to the more complex, whereby gully pot processes and the build-up of sediments are included (Ashley, Hvitved-Jacobsen and Bertrand-Krajewski, 1999). Various approaches to pollutant transport modelling are available within and between SQM's, most critical to variations in water quality outputs is the modelling of sediment transport processes(Schellart, 2007).

Simple deterministic SQM's

In Simple SQM models, pollutants and suspended sediments are moved in the flow of water by advection, dispersion is not accounted for it is considered to have little effect on subsequent variations in water quality. On a timestep basis, the amount of sediment transferable is commonly calculated using the Ackers White equation (Ackers and White, 1973). Sediment can be eroded from the pipe until the sediment store is depleted or the transport capacity is reached; two sediment layers are commonly represented within SQM, the storage layer and active layer. The storage layer can be defined by the user and is generally used to represent consolidated sediments deposited over a longer period. The active layer represents unconsolidated sediments (mostly of organic matter deposited from the dry weather flow). These sediments have a shear strength (Hrissanthou and Hartmann, 1998). This strength must be exceeded before erosion of a sediment will occur. The stored sediment cannot be eroded until the active layer has been removed. In simple SQM's, deposition is often not accounted for in and sediment is held in suspension however pollutants and sediments which are attached to sediments can be partitioned using a settling model which incorporates the use of a tank efficiency factor (Schellart, 2007).

Sewer Model Build, Calibration and Verification

The UPM procedure details model build, calibration and verification steps to aid in the development of sewer quality models which represent reality.

During model build, the use of catchment characteristic data to build a representation of the sewer network, at this stage default values are commonly used for influential water quality variables such as dry weather flow and sediment characteristics. This data includes:

- Land-use characteristics;
- Pipe sediment depth data;
- Point inflow data;
- Storm quality data;
- Physical and chemical sediment characteristics for pipe and surface sediments;
- Dry weather flow quantity and quality data.

Model Calibration

The aim of this procedure is for the shape and dimensions of model hydrographs and pollutographs to represent the system being modelled. Model predictions are compared with observed field data and an adjustment process is undertaken such that default model parameter values are adjusted to values which represent the catchment. Flow data should be fitted before any SQM sub sediment transport sub-model is calibrated as pollutants associated with sediments can cannot be modelled effectively until a sediment transport sub model has been calibrated

The extent to which data is available for calibration of model parameters can determine the accuracy (and usefulness) of the SQM. It is recommended that calibration data be collected at key points in the system i.e. ancillary structures and CSO inflow and outflow locations.

Model Verification

Model verification is carried out during model development with the goal of producing an accurate and credible model. Measured event data is required to evaluate how the model simulates reality in both wet and dry conditions. The

UPMs definition of a 'valid' model is one which obtains acceptable agreement between model prediction and independent field measurements not obtained for calibration.

Sewage Treatment Works Quality Modelling

Sewage Treatment Work Models (STQMs) are used in conjunction with river and sewer models to represent the whole urban catchment. Sewage treatment work performance is assumed to deteriorate during wet weather events if considering the total percentage removal of pollutants through treatment. Conversely, wet weather events have a dilutionary effect on sewerage and thus the concentration of TSS, BOD and NH_4 within final effluent may not differ from average flow conditions. In summary, the effect of storm flows on STW can influence:

- Settling Processes.
- Biological removal processes.
- Solids washout.
- Mechanical problems on the treatment works.

STW models can be generalized into the following categories:

- Dynamic STQMs.
- Reduced-order models.
- Statistical models.
- Time-series models.

Detailed mechanistic (dynamic STQMs) use theoretical equations that describe physical and biological processes. Default calibration parameter values can be used but due to site to site variations; most of these models require calibrating for a given site (Stokes *et al*., 1993). STQMs will typically contain the following sub-models to determine final effluent concentrations of BOD, COD, NH_4, oxidized nitrogen, and phosphorus:

- Activated Sludge.
- Storm Tanks.
- Primary Settling Tanks.
- Final Settling Tanks.
- Trickling Filters.

Reduced-order are simplified versions of the above mechanistic models i.e. nitrification terms may be removed from mechanistic equations where the sewage works does not nitrify. These models may not be as valid as 'detailed mechanistic' models, however, they are as valid as a fully STW model if the effects removed are not significant.

Statistical Correlations models use empirical equations/function relate effluent quality to operating characteristic and influent sewage (Temmick *et al.,* 1993).

Time Series models operate on the principle that the future will represent the past (they use historic time-series data to predict future, they are useful in stable operation conditions but are subject to failing to adequately represent reality (predict effluent quality) when gross changes in plant configurations occur (Novotny *et al*., 1991).

These models follow a similar data collection, model build, calibration and verification procedures as those described for SQMs, the details of which are not considered within the scope of this work and are therefore not presented.

River Quality Impact Modelling

River impact models (RQIMs) allow an understanding of the effects of intermittent wastewater discharges on receiving water quality.

The effects of intermittent discharges on river quality are presented in Section 2.3 Table 2-3. The magnitude of the effect that the aforementioned processes have on DO is related to a number of riverine characteristics, adapted from (Nakamura, 1989):

- Upstream riverine quality – Assimilation capacity of the river is influence by levels of BOD and DO already present within the receiving water.
- River channel slope – Steepness of channels can create turbulence, this can increase the rate oxygen transfer across the air/water interface.
- River channel geometry and roughness – The channel cross-section and water depth can impact turbulence in river, conducive to the occurrence of reaeration.

- Riverine Structures – structures can impact flow velocities and thus water depth; usually having the reduced effect of aeration; thus, creating locations of critical water quality conditions.
- pH – High pH levels increase the proportion of un-ionized ammonia at a given concentration of total Ammonia, however, at higher pH levels, un-ionized ammonia has a reduced toxicity to fish. Ultimately, determining pH levels in a river is critical in understanding the impact of un-ionized ammonia.
- Temperature – River temperatures are also critical to determining the levels of un-ionized ammonia for given concentrations of total ammonia. Higher river temperatures ultimately cause lower DO saturation concentration conditions; reducing a rivers assimilative capacity. Degradation processes also increase at a higher temperature.
- Aquatic Plant Growth – In river vegetation can affect DO levels by two processes related to the time of the day/the amount of sunlight present:
- Photosynthesis adds oxygen to an in-river water column (during daylight hours);
- Plant respiration reduces oxygen levels in the water column (at nighttime hours).

A range of river quality impact models exist that assess the impact of intermittent discharges on receiving waters. Mass-balance models predict wastewater discharge quality with an appropriate quantity of river water to give an estimate of the resulting downstream quality. These types of models do not consider any in-river processes. The models are useful for determinants such as ammonia, this is because the worst impact is likely to be experienced at the point of mixing. These types of models are often used to compare BOD concentrations against standards set to achieve an acceptable DO regime.

Mass balance models include BOD/DO relationships to allow BOD and DO levels to be calculated through time. The models use equations to calculate the DO balance following BOD decay and surface aeration within rivers. These models use relatively simple equations, this allows for the development of analytical solutions and the deployment of numerical procedures to develop solutions, thus the following simplification procedures are usually required:

  - Dismissal and thus non-inclusion of nitrogen transformations.

- The assumption that flow is steady and that the riverine channel is uniform in geometry.
- Dismissal and thus non-inclusion of main oxygen demand processes, at either the riverine bed and/or the water column.

Complex dynamic RQIMs describe the varying quality and flow in a river in response to wet weather events. Differential equations describing the hydrodynamics and water quality processes are solved via the use of numerical techniques. These types of models generally include description of the following processes:

- Pollutant routing – inclusion of advection, dispersion and mixing of pollutants.
- Biochemical processes – inclusions of biochemical degradation processes that will ultimately affect BOD and ammonia.
- Sediment interaction – inclusion of settlement, resuspension, transport, storage and release of sewer derived and river sediments.

As repeated through the UPM, the choice of model complexity is largely determined by the type of problem being analyzed (WaPUG, 1998b).

The use of dynamic RQIMs has progressed rapidly with the development of computer processing power. These models can be used to model a wide range of varying flow conditions and pollutant impacts in complex riverine channel networks. Many of these models operate in one-dimension; flows and concentrations are presumed to be uniform both vertically and horizontally within the water column. Two and three-dimensional models are available however these are increasingly more appropriate and necessary for cases involving estuaries, tidal rivers, stratified river and lakes. It is beyond the scope of this work to consider these models in the context of RQIMs, thus this section discusses one dimensional models only.

Examples of river impact models are:

- MIKE 11 (www.mikepoweredbydhi.com).
- DUFLOW (www.mx-systems.nl/duflow).
- HYDRA (hydramodels.com).
- SALMON-Q (https://arxiv.org).

These models all contain mathematical description models for:

- Hydrodynamic effects.
- Advection-dispersive effects.
- Water quality.
- Sediment deposition modelling.

A hydrodynamic module to model hydrodynamic results are necessary before advection-dispersion or water quality processes can be simulated. Saint-Venant equations are solved using an implicit finite difference scheme to calculate varying flow conditions. The implicit finite difference scheme is also used to solve Fickian advection-dispersion equation; conservation of mass of both dissolved and suspended substances is performed. The advection-dispersion module can also conduct sediment transport equations. The water quality module describes biochemical processes at each specified time and distance step, they are based on empirical equations; this module is normally run simultaneously to the advection-dispersion module. Typical determinands modelled are: BOD; nitrate; temperature; ammonia; DO; sediments and BOD attached to sediments; coliforms; nutrients; chlorophyll-a and toxic pollutants. Sediment deposition modelling describes the erosion and transport of sediment attached to BOD such that the correct simulation of delayed Oxygen demand exerted from the polluted bed sediment; this is critical when trying to predict the impact of intermittent discharged from CSO's (FWR, 2012).

Results from RQIM's are to be assessed in regard with the studies previously appropriate environmental criterion. Results of determinand concentrations are compared with concentration-duration-threshold (CDT) criteria by production of results in terms of summary statistics.

Simplified Urban Pollution Modelling

Detailed deterministic simulation models can be utilized to provide accurate representation of the urban drainage system performance under wet weather conditions. However, they can be somewhat onerous due to the time, effort and computer processing power required to complete multiple runs over the necessary ranges of wet weather conditions. Understandably, compromises are made and the impact of small sub-sets of events are selected and examined, as a result, full understanding of system performance may be lost and the development of appropriate solutions may occur (Dempsey, Eadon and Morris, 1997).

An alternative approach to this problem is to create a simplified model of the urban drainage system and subsequently calibrate this model to a small number of detailed model results; thus, the simplified model may be used for multiple runs. It is accepted that the loss of accuracy is compensated for by the ability to understand the system performance over a greater range of even simulations; thus, greater overall confidence in system performance assessment is attained. These approaches allow for a greater account of variabilities in river conditions, marine conditions, foul quality flow and rainfall. This can enable the development of potential solutions to be evaluated rapidly through the reduction of total model run times. A model specifically recommended within the UPM procedure to achieve this paradigm is 'SIMPOL' (Dempsey, Eadon and Morris, 1997). SIMPOL is a spreadsheet model which represents the elements of the sewer system by tanks, these tanks are conceptually connected to simulate the system configuration. Pertinent to this work is the way in which SIMPOL allows the user to understand the systems environmental impacts. For the case of river flows and concentrations, specification of mean and 5%ile flows and mean 95%ile concentrations are obtained. The model then selects flows and concentrations at random from distributions (typically log-normal for water quality constituents) for pre-user defined rainfall events. Outputs files for each event - including total spill volumes and loads from each discharge structure (CSO tanks and storm tanks) are utilized together with STW outputs (typically six hours' worth of data) and mixed with six hours of river data. The outcome is a prediction of quality concentrations for six hours at the specified event. This process is repeated using different random river flow and quality specifications; allowing for a given storm discharge to mix with different river conditions; this result is used to estimate the quality constituent under analysis (usually BOD in the first instance) exceeded for six hours as a specified return period event (usually one year). The modeler can then compare these results with derived intermittent standards (more readily applicable interpretations of the FIS and percentile standards. If compliance with the relevant standards is not achieved, system adjustments (pass forward capacities and storage volumes) can be made and the simulation repeated;

repetition typically takes less than one minute. Once a solution meets the predefine BOD solutions identified, the process can be repeated with a different quality constituent (Ammonia); in which case BOD stored would be set to zero and with dry weather flow and upstream river concentration changed to represent appropriate ammonia values. The results previously representative of BOD can then be interpreted for Ammonia.

2.6.1.3 PART C – Developing Solutions

Part C of the procedure involves establishing site specific environmental and emission standards. Once established, suitable events are selected for trial against these standards. The planning tools assembled in Phase B of the procedure can then be utilized to predict performance through comparison against the established environmental and emission standards can be performed. Modification to the modelled systems are then trialed until a suitable solution is identified.

Finally, consideration is given as to whether the solution identified could be refined further by the utilization of more complex modelling tools. A decision is taken on whether the cost of building more complex models is necessary in respect of total solution costs, if further investigation can be justified, the study returns to Phase B.

The solution development methodology can be summarized as follows (it applies to discharges to rivers, bathing waters and for meeting amenity standards):

- Establish specific site standards;
- Prepare rainfall event files;
- Estimate the discharge regime;
- Estimate river necessary water quality concentrations;
- Compare with standards;
- Add extra capacity in models;
- Assess design requirements for solids separation;
- Check solution is compatible with other plans;
- Identify improvements needed in data/models.

This process attempts to ensure that adequate protection of riverine aquatic life will be provided by the solutions that are cost effective; do not incur unnecessary costs and are not over or under designed (FWR, 2012).

2.6.1.4 PART D – Consenting and Detailed Design

On completion of the planning study and identification of necessary UDS upgrade measures, under the guidance of the UPM, consent conditions need to be set for the new or modified discharges (NRA, 1994). The process is summarized as follows:

- For existing satisfactory CSOs that are not subject to change, only specific current conditions need specifying.
- For CSOs deemed unsatisfactory due to one criterion, new consent should be used to tighten performance for the failing criterion.
- If CSOs fail two or three criteria, new consent should take account of all requirements.

Any new consents issued must include:

- Overflow locations.
- Overflow type.
- Weir settings.
- Storage requirements.
- Aesthetic performance standards as appropriate to the receiving water uses.

2.6 Integrated Catchment Management

The EU Water Framework Directive (WFD) specifies a sophisticated and holistic assessment of the water quality within a catchment in order to meet environmental and ecological objectives. Integrated catchment management approaches are increasingly being used to address this requirement, utilising a system of integrated models to identify cost and energy effective measures to meet water quality objectives (Benedetti *et al.*, 2010). This Integrated Catchment Modelling approach is based on the use of modelling tools to represent the different components of the catchment system and their interactions i.e. catchment runoff, sewers, treatment works, and receiving waters (Jakeman and

Letcher, 2003). A representation of a typical catchment, conceptualized respective pollutant sources and a ‘combined’ drainage system discharging into a receiving water body is presented in Figure 2-3.

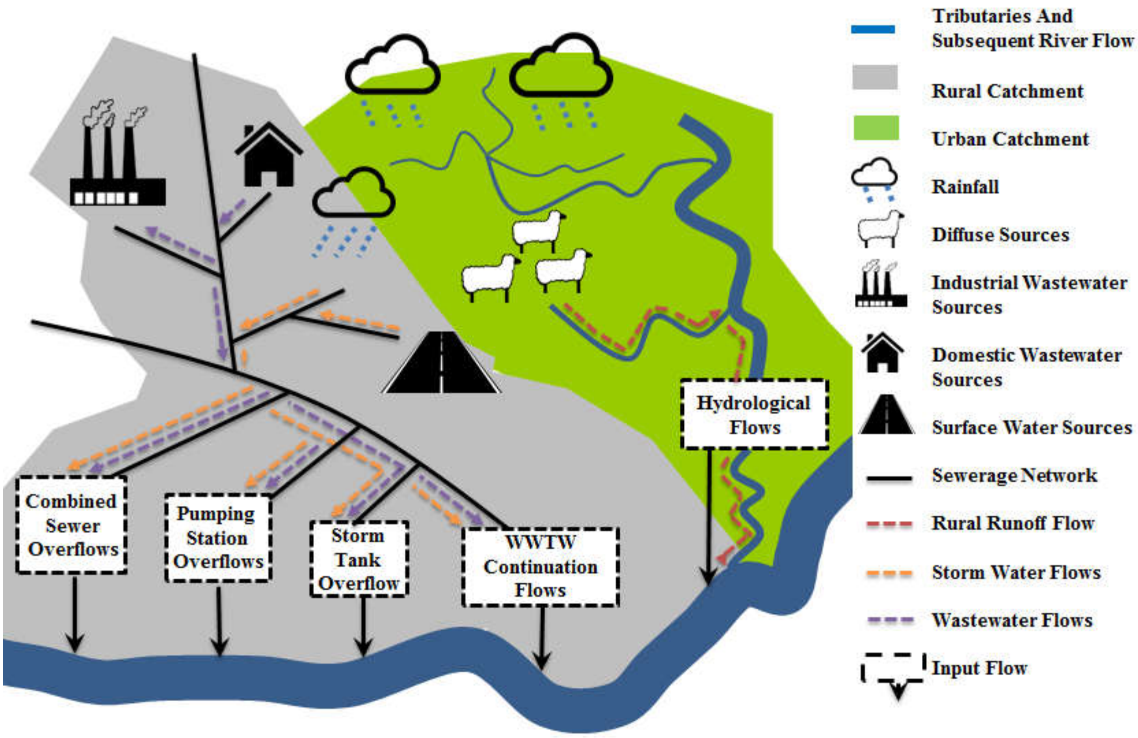

Figure 2-3 Conceptualisation of catchment and inputs into receiving water body (in this example, the river).

In both the urban and rural areas of a catchment, contributing components of flow and water quality can be conceptually separated, in reality they are far from discrete and interact significantly. On the catchment scale, to quantitatively evaluate the impact of urban discharges on a receiving water body, all sources of flows and water quality which contribute to the quality of receiving water bodies must be accounted for; this includes those from the rural ‘upsteam’ areas of a catchment. In these areas, diffuse pollution is derived mainly in the form of pesticides and sediments transported during rainfall events within overland flows from activities such as agriculture, forestry and mining (represented in Figure 2-3 as ‘rural runoff’). The ‘hydrological flow’ component shown in Figure 2-3 incorporates this rural based pollution.

The urban drainage system (often referred to as the sewer system) can be considered as a network of channels, structures and/or underground pipes. In the UK, approximately 70% of sewer system are ‘combined’ that is that the surface water collection system is integrated into the sewerage system, thus both wastewater and storm water flows are conveyed together to the ‘downstream’ waste-water treatment works before being treated and discharged into the receiving water body, during rainfall events. As previously discussed, if the hydraulic carrying capacity of the sewer system is exceeded, storm water and wastewater can be discharged into a receiving water body (as shown Figure 2-3).

The ICM approach allows for the consideration of catchments as one whole system and can be used to assess a combination of factors across different components within a catchment system which could lead to a critical situation (whereby the status of receiving water body becomes compromised), this could not be assessed by focussing on one part of the catchment system only, the approach promotes a catchment wide approach to interconnected environmental issues and consideration of possible future pressures and impacts (Lerner, et al., 2011). ICM is a philosophy underlying the WFD (Mannina and Viviani, 2009), the approach is fundamentally underpinned by the ability to simulate and predict the current and future hydraulic water quality behaviours of each component within a catchment. A schematic interpretation of the integrated catchment methodology is presented in Figure 2-4, for simplicity and understanding; the surface water component has been represented as a separate input to the receiving water model.

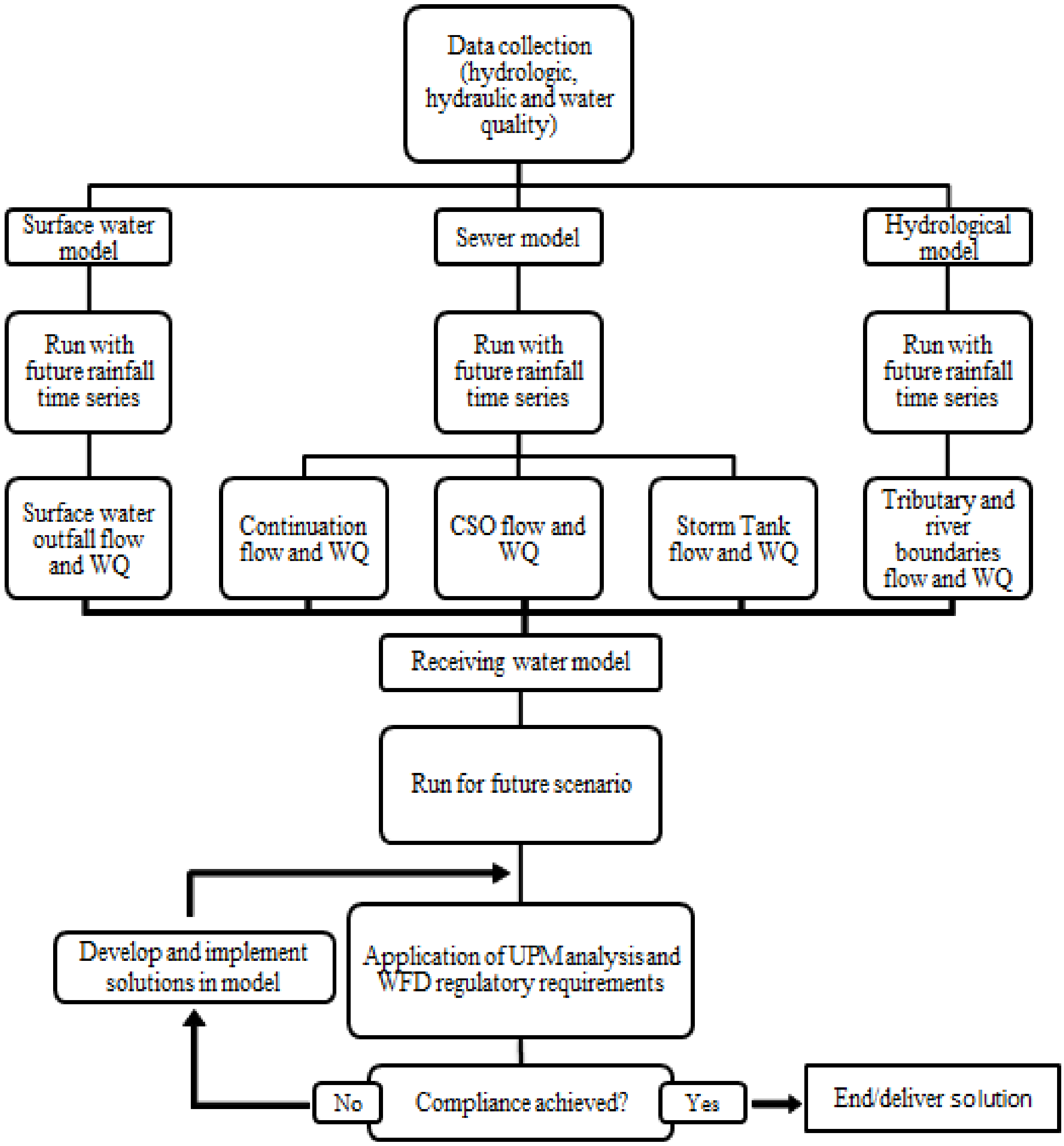

Figure 2-4 Schematic interpretation of the Integrated Catchment Methodology (WWTW inputs are represented as part of the 'continuation flow and WQ' an input into the receiving water model).

Hydraulic and water quality modelling is applied to each catchment component to simulate the behaviour of the integrated catchment system and to account for the effects of transient flow and load characteristics in the sewer, waste water treatment works and receiving river system. Continuous simulations are carried out with different models to ensure that discharge and climatologically changes are taken into consideration and that accumulative loads are accounted for. Following compliance assessment (application of the water quality standards presented in section 2.6.1.1 PART A and in accordance with the WFD standards) solutions are proposed to remediate any failing water courses and these solutions modeled further until compliance with environmental and ecological standards is attained.

2.7 Uncertainty

Models are ultimately mathematical simplifications of reality, this can lead to uncertain model results, it has been suggested that uncertainty elimination is not possible and that uncertainties within models will always be inherently present (Harremoës and Madsen, 1999). With outputs from models utilised in various urban drainage applications, understanding how the impact of model simplifications representing reality is necessary (Morgan and Henrion, 1990). The use of quantitative uncertainty techniques seeks to address this need (Deletic *et al.*, 2012). This section presents a structure with which to describe uncertainty, provides examples regarding the implementation of uncertainty techniques and the associated implications of such implementations within urban drainage modelling.

2.7.1 Classifying Uncertainty

Different methods of classifying uncertainty are presented within the literature (Korving, 2004). Jensen (2002) presented the argument that when model objectives change, uncertainties associate with such a model may also change. Wynne (1992) suggested that model uncertainties can be classified on a spectrum ranging from ignorance to certainty. Harremoes and Madsen (1999) and Korving (2004) used the following system to classify uncertainties within urban drainage systems:

- Ignorance: “We don’t know that we don’t know”, stated by Wynne (1992).
- Indeterminacy: consequence, probability or both are not known for a given event.
- Uncertainty: Important system parameters are known, but the probability distributions of these parameters are not.
- Risk: probabilities of failure can be predicted due to system behaviour being understood.
- Certainty: future system performance is predictable.

When dealing with uncertainties, only those which can be quantitatively and qualitatively described can be examined further, uncertainties classified as ‘ignorance’ cannot be dealt with for they are unknown. Classification of uncertainties is important for it enables the reduction in types of uncertainty that are unexaminable to be removed (Vanrolleghem *et al.*, 2015). Figure 2-5 presents uncertainty types defined by Slijkhuis et al., (1999) and Van Gelder (2000), this uncertainty classification system was used by Korving (2004).

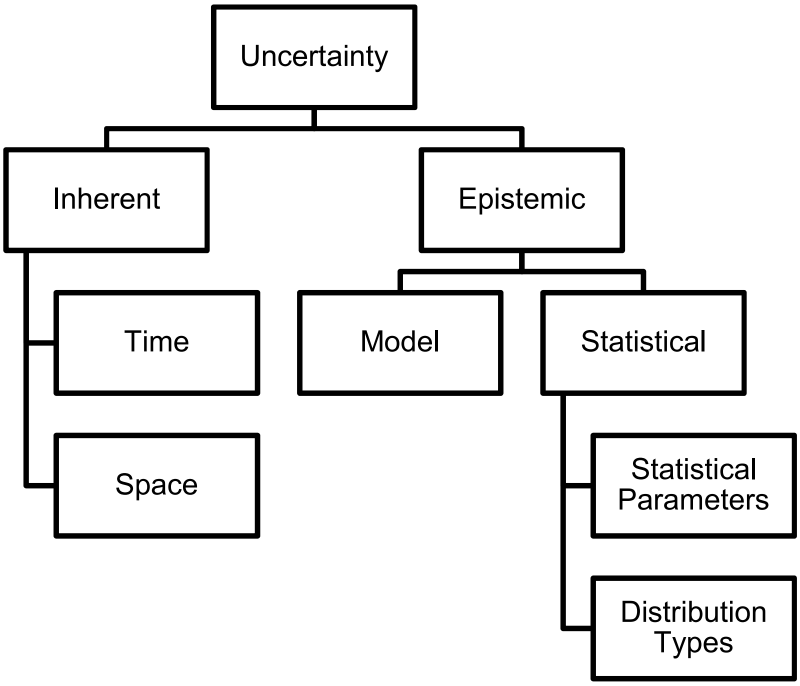

Figure 2-5 Uncertainty classification system according to Korving (2004)

Inherent uncertainty represents the phenomena of randomness, often referred to as stochasticity within natural processes, this is sometimes referred to as ‘natural variability’ (Deletic *et al.*, 2012). Work by Kiureghian & Ditlevsen (2009) represented a similar classification system but utilised different terminology, using the term ‘aleatory’ as oppose to ‘inherent’ to describe uncertainties related to natural variabilities. These ‘inherent’ or ‘aleatory’ uncertainties are found both in the temporal and spatial realm. Inherent time-based uncertainties are fluctuations in processes due to time which cannot be known in advance; these uncertainties are not linked to data availability. In the context of urban drainage modelling, the temporal distribution of a rainfall event would be an inherent time-based uncertainty, an example of a space based inherent uncertainty within the urban drainage modelling process would be the spatial distribution of a rainfall event (Schellart, 2007).

Epistemic uncertainty represents the lack of knowledge concerning the fundamental phenomena associated with the system under observations, model based types of epistemic uncertainty can arise from a lack of understanding regarding physical processes being modelled (Schellart, 2007). Sediment erosion and transport would be a strong example of where epistemic model-based uncertainties are present within urban drainage modelling, these types of uncertainty have been attributed to the complexity of the physical processes involved in their mathematical description (Bertrand-Krajewski, J.L. Barraud *et al.*, 2007; Schellart, A. N. A., Tait, S. J., and Ashley, R. M., 2010). Epistemic statistical uncertainties are often data related, they can be classified as parameter uncertainties or distribution types of uncertainty. Epistemic statistical uncertainties arise when there is insufficient data to accurately define the probability distributions of random variables or the data available fits more than one type of distribution seemingly well (Vezzaro *et al.*, 2013). Sources of uncertainty within urban drainage models have also been classified by Deletic (2010) as follows:

- Model input uncertainties:
    - Input data.
    - Model parameters.
- Calibration uncertainties:
    - Calibration data uncertainties.
    - Selection of calibration input and output data sets.
    - Calibration algorithms.
    - Objective functions.
- Model Structure uncertainties:
    - Errors in model conceptualisation.
    - Inadequate model equations.
    - Inappropriate numerical methods and boundary conditions.

The classification system covers the same sources of uncertainty but defines uncertainty sources in a way which *could* be perceived as more applicable to the practical modelling process. In the classification system, model input uncertainties are those inputs required to run a non-calibrated or calibrated model, they include both random and systematic errors associated with the input data collection process and uncertainty in the calibrated estimates of model parameters. Calibration uncertainties are related to the processes and the data used in the calibration process, dependent on the quality of the data monitoring campaigns used to collect the data and the quality of the instruments utilised to deliver it (Dotto *et al.*, 2010). Calibration uncertainties can also be linked to the choice of calibration variables i.e. pollutant concentrations or loads and the appropriate spatial and temporal resolution of the data e.g. the number of events collected in the monitoring campaign. The selection of calibration algorithms (utilised to find optimal model parameter sets) and the appropriateness of the objective functions are also sources of error associated with the total uncertainty attributed to calibration uncertainties (Refsgaard *et al.*, 2007). Model structure uncertainties are commonly concerned with process conceptualisation, are commonly associated with poorly defined model equations and the inappropriate employment of numerical techniques, therefore it has been suggested that it is inherently difficult to distinguish the attributing source of error between these sources, however, it has been suggested that whilst uncertainties cannot be eliminated, their amplitude and impact on modelling outputs can be quantified (Deletic *et al.*, 2012). Model structure uncertainties have been highlighted in the literature as the most important source of uncertainty (Haydon and Deletic, 2009). With an increased awareness concerning modelling uncertainty and the need to deal with its presence in urban drainage models explicitly argued in the literature (Pappenberger *et al.*, 2006), the need to account for uncertainty within urban drainage modelling studies is clear, even more so if the results of such studies are used in the design of solutions for urban pollution management.

2.7.2 Applications and Implications of Utilising Uncertainty Assessment Techniques within Urban Drainage Modelling.

Uncertainty is present in all urban drainage models (Deletic *et al.*, 2012). It is particularly prevalent in water quality models where natural variations in processes are high, the processes influencing pollutions concentrations are complex and the data used for model development in this area limited (Willems, 2012). The application of uncertainty analysis techniques within urban drainage modelling is limited and challenging, this has been attributed to the complexity and data requirements associated with modelling urban areas; they are often strongly heterogeneous in nature (large spatial variations in soil use, slope, coverage), these complexities and the requirements for large amounts of data have made it difficult to define a universal methodology for the assessment of urban drainage modelling uncertainties (Ballinas-González, Alcocer-Yamanaka and Pedrozo-Acuña, 2016). Considering the classification of uncertainty described in section 2.7.1, a large proportion of uncertainty associated with urban drainage modelling outputs stems from inherent stochastically related uncertainties, this is largely due to the random spatial and temporal nature of rainfall as a model input (Dotto *et al.*, 2014). The understanding of uncertainty related to model input data uncertainties is generally poorly understood (Dotto *et al.*, 2010). Mourad (2005) suggested that when assessing uncertainties associated with calibration, the generation of equally plausible parameter sets can lead to reduced confidence in model outputs. The impact of input data uncertainties has also been examined by Haydon & Deletic (2009), the study assessed the impact of rainfall uncertainties on the performance of non-urban catchment models and suggested that even when using simplistic modelling approaches, the Monte-Carlo simulations required to estimate uncertainty within a practical system can take a significantly long period of time per input variable or model parameter.

Several researchers have investigated natural variability of rainfall, Stransky (2007) used tipping bucket rain gauges to investigate the link between rainfall-runoff processes and rainfall measurement uncertainties; quantifying sources of error, it was suggested that a 30% underestimation of peak flows was possible if rainfall calibration data was not included and that there could be up to a 15% underestimation if systematic errors were neglected. In the context of integrated modelling, Rauch (1998) suggested that a 20% offset in actual to measured rainfall data has an equally significant impact on integrated drainage modelling output results.

The Generalised Likelihood Uncertainty Estimation (GLUE) methodology is an example of a Bayesian approach to assessing uncertainty, its application assumes that prior to the use of quantitative or qualitative information being introduced into the process, model parameter sets which are equally capable of predicting variables of interest must be considered equally likely as simulators of the system under observation (Beven and Binley, 1992). The approach assumes that because all model structures are in a state of error and that because all data sets utilised for calibration will also be subject to error, no one true parameter set can be found. The method is based on the premise that is it be only possible for assessment regarding the likelihood of parameter sets being acceptable simulators of the system, it is therefore suggested that the assignment of likelihood weightings be assigned to model structures and parameter sets on the basis evidence, this evidence can be in the form of both qualitative and quantitate information. Mannina *et al.*, 2006 utilised the GLUE methodology to evaluate appropriate levels of complexity required when modelling sediment erosion processes within sewers, the study utilised twelve rainfall events and corresponding BOD, COD and TSS sampled in Bologna, Italy, to compare the capabilities of six different sediment erosion algorithms of varying complexity. The study concluded that when limited amounts of data are available, the comparison of models with respect to their 'best fitting' capabilities are not important if only limited amounts of data are available. The implications of this approach when utilised to assess uncertainty within complex models were expressed in work by Thorndahl *et al.*, 2008, the work argued that the approach involved significantly high computation costs to carry out assessment on a complex model. Beven and Freer (2001) introduced the argument that the concept of using parameter should be replaced by the concept of 'equifinality', whereby the concept of unique optimal parameter sets may result in equally good fits between model observations and model predictions. Bayesian uncertainty analysis techniques present a statistical framework to the treatment of parameter distributions, the implications of these approaches are that they require large amounts of data, this can make their application within water quality urban drainage modelling limited (Beven and Freer, 2001).

Uncertainty quantification methods whereby input/model parameters described as probability distributions are presented within the literature (Vezzaro *et al.*, 2013). The use of Monte Carlo simulation techniques can be used to apply this type of method, it does not require changes to model structure but becomes increasingly difficult to apply to computationally expensive models, these methods of uncertainty quantification are thus increasingly restricted to simplified models (Sriwastava 2018 – in press).

A method whereby the use of a 'probabilistic' shell built around a deterministic model has been used to quantify the uncertainty in wastewater treatment model design (Benedetti *et al.*, 2006) . The study involved the use of input parameter probability distributions, random sampling of these distributions during each deterministic simulation and the use of independent parallel simulations techniques to derive probabilistic simulation results to be evaluated from economic and environmental perspectives. The study concluded that with recent advances in computation power, the introduction of uncertainty techniques and the availability of well-defined and accepted water quality models, a move from conventionally ‘stiff’ design practises as imposed by emission limits, to transparent and cost-effective procedures provides a more appropriate approach capable of coping with the complexity introduced by integrated water management procedures.

Model reduction techniques involve approximations of a complex model and the subsequent introduction of uncertainty via realisation of the physical system on top of the uncertainty in the complex model (Sriwastava *et al.*, 2018). Schellart (2007) examined the propagation of uncertainty through an integrated catchment model using model reduction and a response database to estimate water quality failures in a receiving watercourse over an extended period. A response database was used to achieve model reduction before application of Monte Carlo simulation to propagate uncertainty through a simplified hydrological model, a computationally expensive sewer hydrodynamic model and a simple river quality model. The study concluded that the overall levels of uncertainty in the ICM inputs had a significant impact on model outputs (water quality failures) and that modelling approaches which do not take into account the uncertainty associated with model inputs and model parameters may results in over or under dimensioned solutions, furthermore the study concluded that with changing external inputs e.g. rainfall and river flows due to climate change, thus better accounting for uncertainty is required.

There are high levels of predictive uncertainty associated with sewer and surface water quality models (Schellart, A. N. A., Tait, S. J., and Ashley, R. M., 2010b). In practise, the propagation of these uncertainties between models, the relative scale of uncertainties derived from individual assumptions/processes and the magnitude of final integrated model predictive uncertainties are seldom considered (Deletic *et al.*, 2012). Combining these factors with the uncertainty associated with input data and field measurements, it could be argued that that the results obtained from such models should always be accepted with caution and evaluated criticality (Ashley, Hvitved-Jacobsen and Bertrand-Krajewski, 1999). Furthermore, the variation and uncertainties within water quality models increase compared to that of hydraulic models making it much harder to transfer experience or default values across catchments, even though they appear similar (Willems, 2010). Work by Dotto *et al.*, (2012) compared the use of different uncertainty techniques, the study concluded that modellers should select a method based on the chosen models structure, number of parameters and the amount of skill/knowledge level the modeller already holds.

2.8 Knowledge Gaps

Whilst it is commonly accepted that the ICM methodology is capable of coping with the requirements of the WFD (Tsakiris and Alexakis, 2012), the most efficient and effective means of delivering the methodology are yet have been agreed. This section describes some of the major problems cited within the literature concerning the application of the ICM procedure, with focus on the use of ‘industry standard’ water quality models currently used within UK utilities to deliver the methodology. This section concludes with a summary of the key knowledge gaps which provide scope for further investigation throughout the remaining chapters of the thesis.

The ICM methodology relies on the use of computer based hydraulic and water quality models to simulate different components of the water system. Computer models for drainage design and analysis emerged in the 1970’s, but complex models only became standard tools of drainage engineers when appropriate computer power became available in the 1980s (Butler and Davies, 2011). Detailed hydraulic models were developed based on accepted mathematical relationships between physical parameters; the models simulate flow propagation in pipes and rivers by solving non-linear partial differential equations i.e. the Saint-Venant equations, with the use of complex numerical algorithms. They involved some method of simplification but could and still can be classified as deterministic: the model is considered to follow definite laws of certainty but not any law of probability. Whilst it is commonly accepted that the application of complex deterministic hydraulic models within the water industry is a successful one, it is also acknowledged that the computational power required to solve such complex algorithms within a business environment is significantly large, thus, model run times can be significantly high. The whole computational time of the integrated model become increasingly prohibitive for carrying out long term simulations of the whole system (Mannina and Viviani, 2010). Furthermore, due to the previous piecemeal approach to catchment modelling, various existing modelling suites represent individual components of the catchment in isolation and with little appreciation for other model component input requirements, this can cause the need for an increased amount of time dedicated to the task of processing data between models or additional data processing steps when exchanging data between models (Refsgaard *et al.*, 2007).

Work by Rauch (2002), suggested that whilst the use of complex models usually improves its ‘realism’, increased complexity of a model can make it increasingly difficult to understand, analyze, pose computational problems and inhibit numerical instability. It has also been suggested that the use of complex models over that of more simplified models does not necessarily improve modelling results since problems and error sources increase with respect to complexity. The integration of individual software components into one system has led to the term ‘intergronsters’. The term has been used to describe integrated models that exhibit ‘constructs that are perfectly valid as software products but ugly or even useless as models’ (Voinov and Shugart, 2013). It is suggested that such constructs ignore the fluid relationships that exist between each component model and reality, the evolving nature of models and their constant need for modification and recalibration.

Furthermore, the integrated model has increased complexity, changes which previously caused impact to relatively contained component models, now propagate through the whole model. This makes complexity difficult to control and goes against the potential benefits of ‘modularity’, whereby efficiency is gained from the independency of component models. This problem becomes further exacerbated by increasing numbers of component models used within an integrated model (Voinov and Shugart, 2013).

The current UK industry standard software package InfoWorks CS is used to model water quality behaviour in the surface water and sewerage systems. The software simulates the transport of suspended sediment and dissolved pollutants by solving the one-dimensional advection-diffusion equation. This equation is formed on the conservation of mass principles and then solved in each conduit or river reach by the Holly-Priesmann method. Different sub models are available to calculate the sediment erosion and deposition in pipes (Zug *et al.*, 1998), however, the most widely accepted sediment model used for erosion and deposition prediction is the Ackers White carrying capacity model (Schellart, 2007;Voogt, van Rijn and van den Berg, 1991). Considering the total computational power required to perform one hydraulic time step simulation coupled with the power to perform an equivalent array of water quality simulations, the use of this complex deterministic ICM model to explore a wide range of design options within an integrated model could be considered to be an inefficient process (Willems, 2010).

The application of complex deterministic models that simulate water quality to a comparable level of detail to that of hydraulic models is much less of a success (Butler and Davies, 2011), the predicative accuracy of these models has been questioned (Deletic *et al.*, 2012). It has been suggested that this lack of accuracy can be attributed to the wide range of physical, chemical and biological processes occurring over a variety of temporal and spatial scales which these models try to describe, many processes of which are currently poorly understood. It has even been suggested that the physical processes in certain water quality models are so complex and catchment specific that it may simply be over ambitious or inappropriate to attempt to represent them in a physically deterministic model (Freni, Mannina and Viviani, 2009). This lack of accuracy is particularly associated with the use of sewer and surface water models, which involve the numerical description of several scientific phenomena related to the fate and transport of pollutants, such as; advection, dispersion, sedimentation and re-suspension. Furthermore, many of the chemical and physical transformations described within these models are dependent on parameters which are very difficult and expensive to quantify accurately or have a high natural variability (Mannina *et al.*, 2012).

The prospect of verifying a pre-calibrated quality model is a less realistic proposition than for a flow model. All models need local data to enable model build, calibration, and verification and it is widely accepted that in general, the accuracy of model outputs can significantly increase with respect to an increase in available data; however, it is often the case that only few measured events are commonly used for such calibration (Mourad, Bertrand-Krajewski and Chebbo, 2005). In practice, data collection is highly resource demanding, budget driven and consequently data are lacking. It has been suggested that according to sewer managers, many water quality models are not cost effective because of the cost of the calibration campaigns and their poor accuracy level compared with that of hydraulic models (Ahyerre *et al.*, 2005).

The use of models as planning, management and design tools is common within the urban drainage field, at present, particularly within industry. Whilst it may appear that water quality modelling software packages are moving forward (offering highly resolute geo-spatial domains in which they can perform an increasingly wide range of analyses), the uncertainty associated with many urban drainage modelling results is often not communicated; this is of significant importance when the outputs of such models are used to plan, manage and design drainage infrastructure which affects various stakeholders (utilities, regulators, the environment and the public). Further still, with integrated analyses becoming increasingly widespread, due to many different urban drainage models providing outputs which are used as inputs into other urban drainage models (often at various temporal and spatial scales) the need to deal explicitly with uncertainty in water quality models is clear (Pappenberger *et al.*, 2006).

2.9 Conclusions

Less complex or 'simple' models are less detailed representations of reality; they generally account for less of the processes that cause variations in hydraulic and water quality behavior and do so at lower spatial and temporal resolutions. This lack of complexity/conceptualization of reality often means that these models require a 'low' amount of computational power to perform one full model simulation, thus model run times are low. Low model run times allows these models to be used more readily in scenario analyses and uncertainty assessments, techniques which provide additional information to the decision-making process when investing in large-scale urban drainage solutions and current assets. There is a 'perceived' lack of accuracy associated with modelling results from simple water quality models and also a lack of quantitative studies within the literature that supports this perception. This is in part due to the cost of expensive water quality data collection campaigns and the subsequent shortages in comprehensive water quality data available for study.

In a business context, the implementation of the ICM methodology is still relatively recent and there is little supporting guidance advising users which types of models are best to support the methodologies deliverance. Furthermore, With the accuracy of results from complex deterministic models questioned, the use of complex deterministic models for water quality prediction and solution development is potentially ineffective and inefficient, if better management decisions are to be made based on ICM results, it seems necessary to evaluate the ‘fitness for purpose’ of the current ‘industry standard’ software tools used to deliver the methodology within industry.

As an alternative to ‘complex’ deterministic quality models, several research groups have developed simple regression based models to predict Event Mean Concentration’s (EMC’s) of pollutants based on catchment and rainfall event characteristics (Kim, Kayhanian and Stenstrom, 2004; Francey *et al.*, 2010; Maniquiz, Lee and Kim, 2010; Dembélé *et al.*, 2011). These models produce results at the event scale, dismissing the inter-event variations of water quality constituents, instead representing them as average pollutant concentration values; in a lumped-temporal manner. They are seldom used within the UK water industry due to the aforementioned ‘perceived’ lack of accuracy associated with such water quality descriptions, yet their utilisation would present decision makers with the opportunity for increased knowledge on the uncertainties present and increased capabilities for scenario analyses within integrated catchment models.

It is in conclusion to this chapter that investigation into the simplification of the ICM methodology without significantly influencing, and potentially decreasing the predictive capacity of the whole ICM process is needed. This thesis therefore proposes that in the context of integrated catchment models, an investigation into the potential use of ‘simple’ water quality models is needed, and that if such a potential is present, a process should be developed which enables modellers to derived knowledge on the uncertainty associated with such model outputs.

Chapter 3 utilises a previously conducted ICM study in the UK, to explore the significance of the representation of dynamic pollution events as mean values within an ICM methodology.

Chapter 3. Evaluating the use of Simple Water Quality models within Integrated Catchment Models

The aim of this chapter is to investigate the effects of reducing the model complexity of the CSO representation from a fully dynamic to an EMC approach on overall ICM model accuracy, subsequently, the chapter looks to establish whether there is potential for the use simple pollutive descriptive techniques to produce CSO spill modelling results within ICM.

From an operational perspective, when utilising an integrated catchment model for river impact studies, the prediction of sewer/surface water intermittent discharge concentrations and loads is the primary objective (Dembélé *et al.*, 2011). The current industry standard complex deterministic models meet this objective by calculating and describing water quality constituents at high temporal and spatial scales. The models generate dynamic descriptions of CSO water quality spills which are then used as inputs to a receiving water model. As an alternative to 'complex' deterministic quality models, several research groups ((Irish Jr *et al.*, 1998; Dembélé, Bertrand-Krajewski and Barillon, 2010; Dembélé *et al.*, 2011) have developed 'simple' water quality models that predict water quality. Many of these models, characterise water quality at the temporal 'event' resolution, and are separated by their calculation processes into site-mean concentration (SMC) and event mean concentration (EMC) models, they have been mostly established and applied by researchers (Gromaire-Mertz *et al.*, 1999). These models are an inherently simplified approach to water quality modelling in that the temporal variability of a spill event is not considered, they instead characterise spill events as an average concentration.

Due to their inherently simplified description of pollutants, these models require low computational power and have low run times, thus they offer increased capabilities for scenario analyses within integrated catchment models. There utilisation remains limited due to a perceived lack of accuracy, especially in the context of integrated catchment models where the impact of characterising intermittent discharges as average concentrations on final receiving water model accuracy is currently unknown. This chapter seeks to answer this unknown in a case study manner, by utilising a previously developed industry standard integrated catchment model and corresponding observed catchment water quality data to evaluate the potential for simple water quality description techniques to be used within integrated models.

The chapter presents results of an ICM study on BOD, NH_4 and TSS water quality parameters conducted in the UK. The data from this water quality collection campaign has been used to define optimum EMCs for a range of CSO spill events and quantify the minimum possible variance between EMCs and observed water quality parameters over each monitored dynamic spill event. These variances are compared to those observed from the use of industry standard complex deterministic modelling tools used within the original ICM study. To define the relative significance of the inherent EMC variance within an ICM study, the hydrodynamic ICM surface water quality model is used to predict river quality parameters using the optimum spill EMCs as inputs. Results are compared to the original ICM model verification study via the direct comparison of observed and predicted water quality parameters at six locations within the receiving waters. A version of this chapter was presented at the 13th international conference of urban drainage 2014 (Norris, Saul and Shucksmith, 2014).

3.1 Case Study Area and Integrated Catchment Model

The case study catchment used for this study is situated in the North-West of England. The ICM approach was used to model the impact of four urban catchments on the river Tame. The study area is on the east side of Manchester, a heavily urbanised city. A total of 37km of the receiving water course – the river Tame - was modelled as part of United Utilities integrated catchment modelling studies in AMP-5. The watercourse is impacted by four combined sewer/surface water networks; Ashton-Under-Lyne, Dukinfield, Hyde, and Denton, referred to as catchments A, B, C and D respectively for the remainder of this work. Each of these catchments intermittently discharges into the river Tame and its tributaries via numerous CSO's during significant rainfall events, 18 of these CSO's across the four sewer networks were highlighted by the Environment Agency as having an 'unsatisfactory' impact on the river Tame, thus these CSO's and 6 downstream river locations were monitored for the water quality parameters; BOD, COD and

TSS. Figure 3-1 shows the location of the catchments and the receiving water course being modelled, Figure 3-2 shows the subsequent schematic representation of the catchment system with the location of monitored and unmonitored CSO's within each sewer.

Figure 3-1 Case study catchment (image taken from google maps) shows four urban catchments (Ashton. Duckinfield, Hyde and Denton) which discharge into the River Tame

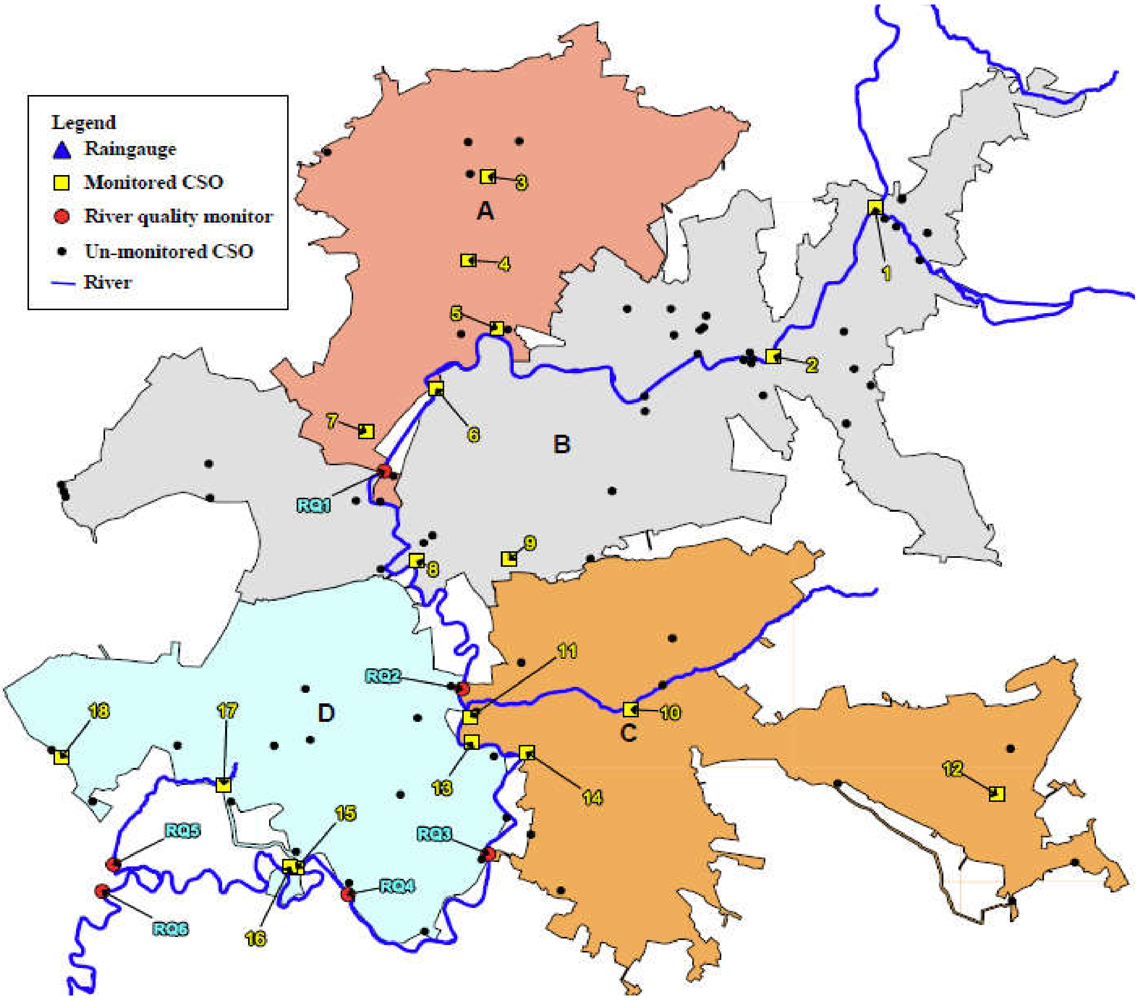

Figure 3-2 Integrated catchment consisting of catchments; A-Ashton-Under-Lyne B –Dukinfield. C –Hyde and D -Denton; Rain gauges; Monitored CSOs, Un-monitored CSOs and the River Tame

The key characteristics of each catchment and each catchment's respective sewer/surface network are presented in Table 3-1.

Table 3-1 Sewer Network Characteristic – UK Sewerage Utility, United Utilities

Sewer Network ID	A	B	C	D
Population Density (p/ha)	47	50	54	32
Catchment Area (ha)	1001	1218	786	1151
Impermeable Area (%)	12	25	31	9
Permeable Area (%)	88	75	69	91
Sewer Length (collectors) (km)	54	75	82	50
Average Sewer Slope (%)	0.024	0.038	0.004	0.016
Monitored CSO's	4	5	5	3
Un-Monitored CSO's	7	32	9	15

3.2 Initial ICM study

The UK water industry operates in Asset Management Plan (AMP) periods, at the beginning of every five-yearly cycle, OFWAT sets water prices following submissions from each utility about what it will cost to deliver their business plan. In AMP5 United Utilities undertook ten integrated catchment modelling studies, this section uses the integrated model and corresponding observed validation data utilized for one of these ICM studies.

The ICM approach is based on the use of modelling tools to represent the different components of the urban drainage system and their interactions (i.e. catchment runoff, sewers, WwTWs, and rivers). Hydraulic and water quality modelling is applied to each component in order to simulate the behaviour of the integrated system and to account for the effects of the transient flow and load characteristics in the sewer-WWTW-river system. Continuous simulations are carried out to ensure that discharge and climatological changes are taken into consideration and that accumulative loads can be accounted for. Prior to the application of the model as a decision-making tool, model build, calibration and verification processes were carried out to the standards expressed in the following UK guidance documentation:

- Code of Practice for the hydraulic modelling of sewer systems (WaPUG, 2003).
- Code of Practice guide for the water quality modelling of sewer systems (WaPUG, 2006).
- River Modelling Guide (WaPUG, 1998b).
- River Data Collection Guide (WaPUG, 1998a).
- Urban Pollution Management Manual (FWR, 2012).

The documents provide a summary of current best practice in the UK at present and provide a framework in which to carry out sewer hydraulic and quality modelling. The WaPUG group was formed in 1982 as an 'advisory group for Urban Drainage', it became the Chartered Institute for Water and the Environment (CIWEM) urban drainage group in 2009, it is run by a committee to reflect its members within the urban drainage. The integrated catchment model and its individual model components were built in accordance with these guidance documents and were passed as suitable by the Environment Agency as appropriate for the design of solutions aimed at managing Urban Pollution. A description of the component model builds, calibration and verification provided by United Utilities and used within the study is presented in the following sections, in line with the scope of the work, full detailed description has been applied to the water quality components of the sewer model, reviews and of other models and their respective calculation methods are also presented.

3.2.1 Hydrological Model

Hydrological modelling provides the rural inflows to the hydraulic models in order to calculate flows and water levels along the river channel. The RAM rainfall-runoff model, developed by DUFLOW (version 3.8.5.0) was employed for this purpose (IHE Delft, 1995). RAM is a physical-deterministic model that simulates the surface runoff by calculating the losses from precipitation and delays in runoff. In the RAM model, a division into types of surfaces is made in view of the differences in rainfall-runoff processes (i.e. open water surface, paved surface, and unpaved surface). The processes that can be modelled in RAM include infiltration into the soil moisture, percolation into the groundwater, groundwater discharge into the drainage system, interaction between saturated and unsaturated zone, and process of leaching and runoff of nutrients.

The RAM rainfall-runoff modules are of strong empirical nature. Therefore, the parameters in the model usually do not have a direct physical meaning. Typical values of these parameters are usually used and calibrated based on the measured discharges. A specific Rainfall-runoff (RAM) model was developed for the River Tame’s hydrological catchment. A single RAM model was developed with an area equal to the rural catchment area, calculated by subtracting the urban area included in sewer models from the total catchment area. In the hydrological catchment the aim of the modelling process was to use a single rain gauge to develop a single set of model parameters to represent the hydrological characteristics of the catchment. The model parameters were verified by comparison of simulated runoff against an appropriate river gauge records. These parameters could then be applied to simulate runoff from detailed rural sub-catchments which excluded the urban areas represented in sewer and surface water models. These simulations took rainfall variability into account by employing multiple rain gauges based on a Thiessen polygon distribution, modified to take account of topography, the Thiessen polygon distribution is a simple and practical method for computing rain gauge station weights. The runoff generated was then introduced into the river hydraulic models, in conjunction with sewer and surface water runoff generated in the sewer/surface water models, and a final comparison made against the EA’s river gauge records. In addition, it was found necessary in some cases to apply seasonal hydrological parameters to get satisfactory matches through the year. Evaporation data from Met Office Rainfall and Evaporation Calculation System (MORECS) square 106 was applied in the models. The MORECS method provides estimates of evaporation, soil moisture deficit and effective precipitation under British climatic conditions, further information on the science behind this method and system is presented in (Hough and Jones, 1997).

The RAM hydrological model for the River Tame was calibrated against the available flow measurements at EA river gauging stations. Calibration of the model was performed using trial and error adjustments of selected model input parameters, model parameters were verified through comparison of simulated and observed flow measurements.

Time series of flows at the head of the catchment river, and additional lateral inflows, were generated using the hydrological model described above. The hydrological catchment was initially subdivided based on the FEH CDROM catchment watersheds technique, further information on this technique is described in the Flood Estimation Handbook (Centre for Ecology & Hydrology (formerly the Institute of Hydrology), 1999). Using this approach, the river Tame hydrological catchment was divided into 6 sub-catchments. Some of these sub-catchments were further sub-divided into smaller areas to assign the runoff flows more precisely based on topography and the locations of point discharges from the urban sewer, surface water and WwTW assets. The calibrated RAM model was applied to each sub-catchment to simulate the flows from the rural areas based on historical rainfall data. The time series of simulated flows from the sub-catchments and tributaries were used as hydraulic input to the river model.

3.2.2 Surface/Sewer Model

The four sewer/surface models were built using the complex deterministic software package InfoWorks CS version 12.5 (Innovyze, 2011, http://www.innovyze.com/). The models have been built and maintained by various UK consultants on United Utilities service framework over AMP periods 3 to 5, the initial build date of the models is unknown, in part because InfoWorks CS is a later version and update of the software Hydroworks, which was developed by merging previous models built in FLUPOL and MOSQITO (Ashley, Hvitved-Jacobsen and Bertrand-Krajewski, 1999). Within InfoWorks CS, the modelling of pollutants is fully conservative, there is no interaction between pollutants and their environment, or between one pollutant and another. InfoWorks CS includes the following modules used to describe water quality processes in the surface/sewer system:

- Solids surface build-up module;
- A gully pot build-up module;
- A surface wash-off module;
- A pollutant transport, sediment erosion and deposition module (three parts within a conduit module).

With this chapter's focus being on the accuracy of results generated from deterministic sewer quality modelling packages within an ICM study, the water quality modules utilised within InfoWorks CS (the package utilised in this ICM study) and their scientific description have been described in depth, other deterministic sewer water quality models are available which could have been used to provide inputs into the receiving river impact model within the Integrated Catchment Model used for this study such as the United States Environmental Protection Agencies Storm Water Management Models (US-EPA, www.epa.gov) and DHI Water and Environment model MOUSETRAP (www.dhi.dk/mouse).

SWMM is a distributed discrete time simulation model. SWMMs surface build-up module utilises Sartor and Boyd's nonlinear function of dry days (1972) to estimate build up for different land uses on the catchment surface; different functional options (power, exponential and saturation) are available to the modeller. For surface wash-off, SWMM offers a more simplified method of calculation. Research by Ammon (1979) concluded that whilst sediment transport theories are attractive to users, field data requirements to derive parameters involved in sediment transport theory are significantly large, SWMM therefore offers different empirical models to represent wash-off of pollutants from the catchment surface; exponential wash off, rating curve wash-off and EMC wash off. For pollutant transport, SWMM offers numerical solution of the 1-D advection-dispersion equation, the model further assumes complete mixing within conduits via the form of a continuously stirred tank reactor model. MOUSETRAP utilises a surface runoff quality module capable of simulating the build-up and wash-off of pollutants, a sediment transport module with the option of four different transport equations, an advection-dispersion module to compute pollutants advection and dispersion through the sewer network and a water quality process module to compute processes within the sewer network.

InfoWorks CS Modelling

InfoWorks CS combines geographical analysis with a relational database to provide an environment in which modellers can simulate key elements of wastewater, storm water and/or combined or sewer systems within a single environment. The software utilises a time-series simulation engine to perform numerical solutions in a time-stepping manner. Interactive views of model networks are provided by a geographical user interface, users can view long sections, geographical plan views, spreadsheet and time varying geographical data. Underlying network model data is stored in a database categorised by network nodes, link and sub-catchment network objects.

Network Model Data

Networks nodes are used to represent manholes, storage structures, ponds, outfalls and breaks. Nodes must be joined by a link, which represents either:

- the physical connections between two nodes: either a close pipe or an open channel, or
- A control, representing a weir, pump, or other flow device.

Sub-catchments represent the physical area with which a manhole or other inflow node collects water, each sub-catchment can be defined as collecting the following types of water: storm (rainfall collection); foul (wastewater collection); combined (rainfall and wastewater collection) and overland (overland floodwater collection). How a sub-catchment behaves during simulation is influenced by default or user defined runoff and land use characteristics.

Links can be used to represent and describe the following network objects and object characteristics respectively: conduits; culvert inlets; culvert outlets; flap valves; flumes; head discharge; flow efficiencies; orifice's; pumps; rivers; screens; siphons; sluice's; user defined controls; weir and river shapes.

Model Simulation

The behaviour of the network under conditions is modelled by running simulations. Simulations test the effects of a given flow of water through the network over a prescribed period of time, this allows modellers to understand the behaviour of the network under given rainfall patterns. Simulation parameters govern how InfoWorks CS performs model calculations in the hydraulic and water quality simulation, it is not normally necessary to amend the network simulation parameters; default values have been chosen for optimum simulation performance regarding computation cost. The data for simulations comes from the definition of an event - hydrological and hydraulic data that varies with time - which contains data such as rainfall records or a prediction of domestic wastewater inflow. The software performs full solution modelling of:

- Backwater effects and reverse flow.
- Ancillary structures.
- Trunk sewers.

▪ Conduits (pipes) and respective conduit connections.

InfoWorks CS Water Quality Modelling

The InfoWorks CS Water Quality model simulates the build-up of sediment in the network and the movement of sediment and pollutants through the drainage system during a rainfall event. The hydraulic module calculation process takes place before the water quality model calculation process at each timestep as outputs from the hydraulic model are used in the water quality calculations.

The modelling process takes place in two stages; model initiation and model simulation. The initialisation stage involves carrying out initialisation runs to find a steady state for the network. These runs will often be dry weather flow runs to generate an initial state in dry weather conditions. In the simulation stage, users can apply different rainfall events to the initialised model. InfoWorks CS recommends a build-up period prior to each modelling simulation to let the surface sediment and pollutants reach a steady state. In the simulation stage, application of different rainfall events is used to initialise the model.

InfoWorks CS allows users to model up to nine different pollutants and two different sediment fractions. There are five named pollutants and four additional user defined pollutants. The named pollutants are: Biochemical Oxygen Demand; Chemical Oxygen Demand; Total Kjeldahl Nitrogen; Ammoniacal Nitrogen and Total Phosphorus. Each pollutant can be modelled as a dissolved pollutant, or as pollutant attached to one or both sediment fractions using a potency factor (Ammoniacal Nitrogen can only be modelled as a dissolved pollutant). The two sediment fractions can be modelled:

- Completely independently, with no interaction between them; or
- as dependent fractions, where average sediment parameters are calculated and then a single calculation carried out for the combined sediment.

InfoWorks CS includes the following modules used to describe water quality processes in the surface/sewer system:

- Solids surface build-up module.
- Gully pot build-up module.
- Surface wash-off module.
- Pollutant transport module (part of the conduit module).
- Sediment erosion and deposition module (part of the conduit module).

InfoWorks CS Surface Build-Up Module

In dry weather conditions, sediment builds up until a steady state is reached on catchment surfaces, a layer of active sediment also builds up in network conduits. This active sediment can be transported by flows in the network. Active sediment sits on top of a fixed layer of bedded sediment that does not change during the simulation. Inflows of sediment and pollutant that follow a 24-hour pattern can come from areas of population (wastewater events) and industrial sources (trade events). Inflows of sediment and pollutants that do not follow a 24-hour pattern, such as weekly tank flushing at an industrial plant, can be applied using associated pollutant profiles and inflow hydrographs.

During a storm event, dry weather inputs continue to enter the network, however rainfall generates runoff from the catchment and into the network; this causes sediment to be eroded from the catchment surface and washed into the network. Dissolved pollutants are also flushed into the system by surface runoff and increased flows cause increases in the erosion and transport of sediments.

The solids surface build-up module within InfoWorks CS calculates sediment build up prior to and during the period of simulation, this governs the amount of sediment than can be washed into the network. The build-up equation (Equation 3-1) is used to determine the mass of sediment build-up only.

Equation 3-1

$$\frac{\mathrm{dM}}{\mathrm{dt}} = \mathrm{Ps} - (\mathrm{K_1} * \mathrm{M})$$

Where:

M = the mass of deposit per surface unit (kg/ha)

Ps = the build-up factor (kg/ha.day)

K_1= the decay factor (0.08/day) default deduced from empirical calibration.

The maximum surface mass available is given by:

Equation 3-2

$$M_{max} = \frac{Ps}{K_1}$$

Where:

M_{max} = maximum surface mass available (kg/ha)

Ps = the build-up factor (kg/ha.day)

K_1= the decay factor (0.08/day) default deduced from empirical calibration.

The maximum surface mass available calculated in Equation 3-2 is never exceeded, user defined limits can be applied to stop sediment build-up if required. InfoWorks CS calculates the build-up of sediment and the erosion of sediment in parallel for each timestep. Both these calculations begin with the initial sediment mass at the start of the timestep. The sediment mass at the end of a timestep is calculated by projecting the mass without erosion less the amount of eroded sediment; both these amounts can be calculated by integration of the build of equation (Equation 3-1). The mass of deposit is given by:

Equation 3-3

$$M_0 = M_d e^{-K_1 NJ} + \frac{Ps}{K_1}(1 - e^{K_1 NJ})$$

Where:

M_0 = the mass of sediment at the end of the build-up period or the projected mass at the end of the timestep (kg/ha)

M_d = the initial mass of sediment deposit (kg/ha)

K_1 = the decay factor (0.08/day) unless otherwise specified by the user

NJ = the duration of the dry weather period or timestep length (days)

P_s = the build-up factor (kg/ha.day).

During a rainfall event, surface mass is dependent on the erosion rate and build-up equation (Equation 3-1) using the first order numerical Euler approximation method. Surface build-up changes with respect to the surface build-up factor in Equation 3-1, if not otherwise specified, InfoWorks CS uses the factors presented in Table 3-2 with respect to sub-catchment land-use.

Table 3-2 InfoWorks CS default surface build-up factors

Land Use	Surface Build--up Factor (kg/ha/day)	Origin
Residential (dense)	25	Desbourdes
Residential	6	Desbourdes
Town Centre	25	US Calibration (EPA)
Industrial	35	US Calibration (EPA)
Mixed Suburban	6	Debourdes

Gully Pot Build-Up Module

The gully pot module calculates the initial pollutant concentrations in gully pots before and during a simulation. The calculation is carried out for each sub-catchment. Only dissolved pollutants are modelled in gully pots. Sediment build-up is not considered. The basic hypothesis underlying pollutant build-up is the time-linear accumulation of each pollutant in a gully pot. InfoWorks CS uses the same build-up equation (Equation 3-1) to calculate build-up during the build-up time period and for each timestep during the simulation, actual concentrations of each pollutant are calculated by:

Equation 3-4

$$PG_n(t) = \frac{((C + M * ND) * V_g}{1{,}000{,}000}$$

Where:

$PG_n(t)$ = dissolved pollutant mass at timestep t (kg)

C = initial pollutant concentration (mg/l)

M = gradient of linear accumulation (mg/l days^{-1})

ND = dry weather period or timestep length (days)

V_g = gully pot volume (m^3).

The gully pot volume for each sub-catchment is given by:

Equation 3-5

$$V_g = D_g * A$$

Where:

V_g = gully pot volume (m^3)

D_g = gully pot depth (m)

A = runoff area of the respective runoff surface for the gully pot under consideration (m^2).

Surface Wash off Module

InfoWorks CS calculates the amount of sediment and pollutant entering the system for each sub-catchment at each water quality timestep. The surface wash off and gully pot flushing calculations are completely independent. The following calculations take place:

- the wash-off of sediment from the surface and the resulting inflow of each attached pollutant based on their potency factors. Wash off is taken from the effective impermeability; and,
- the amount of each pollutant flushed from the gully pots.

The surface wash off model is based the Desbordes Model (a single linear reservoir runoff routing model) (Desbordes and Servat, 1983). InfoWorks CS assumes that the pollutant flow at the sub-catchment outlet (node) is proportional to the quantity of pollutant dissolved or in suspension in the storm water present on the sub-catchment, InfoWorks CS performs the following calculation procedure:

- the amount of sediment eroded from the surface and held in suspension in the storm water (the Total Suspended Solids). This erosion is proportional to rainfall intensity;
- the amount of sediment washed into the drainage network using the single linear reservoir routing model;
- the amount of each pollutant attached to the sediment entering the drainage network. This is also proportional to rainfall intensity.

Sediment Erosion

The mass of sediment eroded from the sub-catchment is a function of the rainfall intensity and the mass of deposit on the ground:

Equation 3-6

$$\frac{dM}{dt} = K_a * M(t) - f(t)$$

Where:

M(t) = mass of surface-deposit pollution per unit area (kg/ha) at time *t*

Ka = the erosion/dissolution factor related to rainfall intensity (-)

f(t) = the pollutant flow at time t (kg/(ha).

Sediment Wash off

InfoWorks CS calculates sediment wash-off using values for runoff calculated with the Desbordes runoff. The Desbordes model's basic hypothesis is that of the single linear reservoir coupled with the assumption that the flow at the catchment outlet is proportional to the volume of storm water present on the catchment. The calculation for sediment wash-off uses the runoff from Runoff Surface 1 and Runoff Surface 2 defined in the land use definition, these are both impervious surfaces, runoff surface 1 is the road surface and runoff surface 2 is the roof area:

Equation 3-7

$$Me(t) = k * f(t)$$

Where:

Me(t) = the mass of the pollutant dissolved or suspended pollutant (kg/ha) at time (t) per unit area.

k = linear reservoir coefficient (s^{-1})

f(t) = the pollutant flow at time t (kg/(ha.s).

If the simulation uses the final state of another simulation to provide the initial state of the current simulation, the initial total suspended solids (TSS) outflow per surface unit is calculated from:

Equation 3-8

$$f(0) = \frac{Fm(0)}{C * Ar}$$

Where:

$f(0)$ = initial TSS outflow (kg/(s.ha))

$Fm(0)$ = the TSS flow (kg/s)

C = proportion of sub-catchment area that is impermeable (-)

Ar = sub-catchment area (ha).

Attached Pollutants

The mass of each pollutant attached to the sediment washed into the system is calculated using potency factors. The potency factors depend on the rainfall intensity. These potency factors (*Kpn*) relate surface mass of sediment to surface mass of pollutant and are calculated using the potency factor equation:

Equation 3-9

$$Kpn = C_1(IMKP - C_2)^{C_3} + C_3$$

Where:

Kpn = Potency factor (-)

IMKP = maximum rainfall intensity over a 5-minute period (mm/hr)

C_1, C_2, C_3 = coefficients (mm/hr).

Equation 3-9 shows that the more intense the rainfall, the more significant the proportion of mineral matter becomes. InfoWorks CS assumes that the potency is constant throughout a sub-event. The coefficients used in the potency factor equation are entered via a surface pollutant editor related to the type of land use being modelled, all surface potency factors are constant throughout a given simulation. InfoWorks CS calculates the mass of pollutant attached to the washed off sediment using:

Equation 3-10

$$fn(t) = kpn * fm(t)$$

Where:

fn(t) = pollutant flow (kg/(s.ha) at time t

kpn = potency factor (-)

fm(t) = TSS flow at time t (kg/(s.ha).

During a simulation, the following calculations are made at every timestep for surface wash off:

1. Calculation of the erosion rate (kg/(ha.s)). The erosion equation is written:

Equation 3-11

$$\frac{dM}{dt} = -K_a M(t)$$

Where:

M = erosion rate (kg/(ha.s))

K_a = rainfall erosion coefficient (-)

M(t) = erosion rate at time t (kg/(ha)).

On integration of the erosion equation, the erosion rate between time *t* and time *t + dt* is calculated from:

Equation 3-12

$$E = M(t) * \frac{(1 - e^{K_d dt})}{dt}$$

Where:

E = erosion rate during timestep (kg/(ha.s))

M(t) = erosion rate at time t (kg/(ha.s))

K_d = erosion coefficient (-).

2. The surface build-up (kg/ha) between t and time *t* + *dt* using Euler approximation to the build-up equation is given by:

Equation 3-13

$$B = \frac{(kP_s - K_1) * M(t)dt}{86400}$$

Where:

B = surface build-up (kg/ha)

k and P_s = build-up coefficients (-)

K_1 = linear reservoir coefficient (-)

M(t) = erosion rate at time t (kg/(ha.s))

86400 (seconds in 24 hours).

3. Calculation of the residual surface mass (kg/ha) for use at the next time step using:

Equation 3-14

$$M(t + dt) = M(t)e^{-K_a dt} + B$$

M(t) = erosion rate at time t (kg/(ha.s))

K_a = rainfall erosion coefficient (-)

B = surface build-up (kg/s).

4. Calculation of the TSS outflow per active surface unit. The expression for TSS outflow is obtained by substituting the reservoir equation $M_e = Kf(t)$ into the continuity equation:

Equation 3-15

$$\frac{dM_e}{dt} = E - f(t)$$

Where:

M_e = the mass in solution per unit area (kg/ha)

E = erosion rate (kg/(ha.s))

$f(t)$ = TSS flow per unit of active surface at time t (kg/(s.ha)).

By integration, the TSS outflow per active surface unit is written:

Equation 3-16

$$f(t + dt) = f(t)e^{\frac{-dt}{k}} + \left(1 - e^{\frac{-dt}{k}}\right) + (1 - e^{-k_a dt})M(t)/dt$$

Where:

$f(t)$ = TSS flow per unit of active surface (kg/(s.ha))

k = linear reservoir coefficient (-)

k_a = rainfall erosion coefficient (-)

$M(t)$ = the mass of surface-deposit pollution (kg/ha).

5. Calculate TSS outflow per sub-catchment:

Equation 3-17

$$Fm(t) = C * A_r * f(t)$$

Where:

$Fm(t)$ = TSS outflow per sub-catchment at time t (kg/(s.ha))

C = the proportion of sub-catchment area that is impermeable (-)

Ar = the sub-catchment area (ha)

f(t) = TSS flow per unit of active surface at time t (kg/(s.ha)).

The pollutant outflow per sub-catchment can thus be calculated by:

Equation 3-18

$$Fn(t) = kpn * C * Ar * f(t)$$

Where:

Fn(t) = the attached pollutant flow (kg/s)

kpn = potency factor (-)

C = the proportion of sub-catchment area that is impermeable (-)

Ar = the sub-catchment area (ha)

f(t) = TSS flow per unit of active surface at time t (kg/(s.ha)).

Gully Pot Flushing

The Gully Pot model within InfoWorks CS describes the method for calculating the amount of dissolved pollutant removed from each gully pot at each timestep during a rainfall event. The Gully Pot model represents the amount of dissolved pollutant washed into the system from the gully pots by runoff from the road surface. The model uses the runoff value calculated by the hydraulic engine for Runoff Surface 1 defined in the Land Use Definition. By convention, Runoff Surface 1 is the road surface. The underlying assumption is even mixing of the pollutant mass in the gully-pot and resulting from surface wash-off, the resulting pollutant flow depends on the inflow from the runoff module:

Equation 3-19

$$P_n = F_n(t + dt) * dt + PG_n(t)$$

Where:

P_n = total pollutant mass (kg)

$F_n(t + dt)$ = dissolved pollutant inflow (kg/s)

dt = timestep (s)

$PG_n(t)$ = pollutant in gully at time t (kg).

Equation 3-20

$$F_n(t+dt) = \frac{Q(t+dt)}{(Q(t+dt) + \frac{V_g}{dt})} * \frac{P_n}{dt}$$

Where:

$F_n(t + dt)$ = dissolved pollutant inflow (kg/s)

Q (t + dt) = runoff from road surface at time t (m^3/s)

P_n = total pollutant mass (kg)

dt = timestep (s)

V_g= volume of gully (m^3).

Equation 3-21

$$PG_n(t+dt) = P_n - F_n(t+dt) * dt$$

Where:

$PG_n(t + dt)$ = pollutant in gully at timestep (kg)

P_n = total pollutant mass (kg)

dt = timestep (s)

$F_n(t + dt)$ = dissolved pollutant inflow (kg/s).

Note in current model no dissolved pollutant enters the gully pot from the road surface therefore $F_n(t + dt)$ input to the P_n equation is always zero.

In the current model, no dissolved pollutants enter the gully pot from the road surface, therefore $F_n(t+dt)$ input to the P_n equation is always zero.

Initial values for sediment mass on the catchment surface can be set by the user or default values provided by InfoWorks CS. Users can model the build-up of sediment during the dry spell prior to a simulation, once the simulation starts, alternating dry weather periods and spells of rainfall can be utilised, during dry weather, build-up of sediment and pollutants continues, during a storm, sediment and pollutants enter the drainage network, build-up continues during storms.

Conduit Model

The conduit model is used to calculate the transport of suspended sediment and dissolved pollutant, and the erosion and deposition of sediment, in conduits. The transport process and the sediment erosion and deposition process are solved separately within each time step.

As with the hydraulic conduit model, a conduit is represented as a conceptual link of defined length between two nodes in the network. Control structures are treated as links of zero length in which no erosion or deposition takes place, It is assumed that:

- The flow is one-dimensional in the conduit;
- The concentration of any suspended sediment and dissolved pollutant is fully mixed across the section of the conduit;
- The suspended sediment and dissolved pollutants are transported along the conduit with the local mean velocity of the flow;
- Dispersion of the suspended sediment and dissolved pollutant along the conduit is negligible;
- Erosion of sediment from the bed is instantaneous;
- Deposition of suspended sediment depends on a settling velocity calculation; and,
- Deposition of suspended sediment does not affect the hydraulic calculations.

Transport

The equation describing the transport of the suspended sediment and the dissolved pollutant is based on conservation of mass. With the assumptions listed above, this leads to the one-dimensional advection equation as described in, for example, Cunge J A et al (1980). It is written:

Equation 3-22

$$\frac{dc}{dt} + u\frac{dc}{dx} = 0$$

Where:

c = concentration (kg/m^3)

u = the flow velocity (m/s) (obtained from the hydraulic simulation)

t = time (s)

x = the spatial co-ordinate (m).

The carrying capacity of the flow is calculated using one of the three erosion/deposition models available in InfoWorks CS (Ackers and White, 1973; Zug *et al.*, 1998; Bouteligier, Vaes and Berlamont, 2002). The advection equation is solved in each conduit by the Holly-Preissmann scheme (Holly F.M. & Preissmann A., 1977)

Sediment Erosion and Deposition

InfoWorks CS supports three different models for calculating erosion and deposition in pipes. These models are:

- The Ackers White Model ((Ackers and White, 1973)
- The Velikanov Model (Zug *et al.*, 1998)
- The KUL Model (Bouteligier, Vaes and Berlamont, 2002)

The following assumptions and limitations apply to erosion and deposition of sediment:

- suspended sediment is assumed to be well mixed;
- erosion of suspended sediment is instantaneous;
- deposition is based on settling velocity;
- cohesive forces are ignored; and,
- no deposition is allowed to occur if the total sediment depth (active plus passive layer) is greater than a user defined percentage (up to 80%) of pipe depth.

Sediment

In InfoWorks CS, sediment in pipes is treated differently by the hydraulic model and the water quality model. InfoWorks CS models two different layers of sediment in pipes in a drainage system.

The two sediment layers are:

- Passive Layer - the passive layer is fixed throughout a simulation.
- Active Layer - sediment from the active layer can be eroded, transported, and deposited during a water quality simulation

If the sum of the passive and active layers is greater than 80% of the conduit height, no more deposition of the active layer can occur.

InfoWorks CS provides the option of feeding back changes in the depth of the active layer during a water quality run to the hydraulic simulation engine, so changes in the sediment depth affect the hydraulic calculations. Alternatively, these changes can be ignored and only use the passive layer used for hydraulic calculations.

If the active layer for hydraulic runs is not included in calculation, InfoWorks CS recommends the use of a lower value for maximum sediment depth (10%) to stop the sediment depth recognised by the hydraulic model becoming significantly different from that used by the water quality model.

Passive Layer

The passive layer of sediment is considered to be fixed and remains unchanged during any simulation. It effectively acts as a constriction on the pipe. The depth of the passive layer is set using the sediment depth field for each conduit. Alternatively, users can define a set of pipe sediment data and include it in a run. If you define pipe sediment data and include it in a run, the pipe sediment data overrides values in the Sediment Depth field. Pipe sediment data is most commonly used to adjust the passive layer, and so places restrictions on the maximum depth of the active layer during water quality simulations, thus pipe sediment data can only be used in a water quality simulation.

Active Layer

The active layer is made up of mobile sediment that can be eroded, transported, and deposited during a simulation. The active layer is made up of one or two sediment fractions that can have different characteristics. These sediments are referred to as Sediment Fraction 1 (SF1) and Sediment Fraction 2 (SF2). Each sediment fraction is defined by two parameters:

- d_{50} - the average sediment particle size (default value 0.04mm); and,
- Specific gravity - the gravity of the sediment fraction (default value 1.7).

These parameters can be user specified in the surface pollutant editor; if left unchanged, the aforementioned defaults are used in water quality simulations.

The maximum depth for the Active Layer is calculated as the maximum sediment depth less the depth of the passive layer. Depths of the Passive Layer can be altered to the maximum depth of the Active Layer. This is achieved by setting new values for the sediment depth field for each conduit. A more practical alternative is to define a set of pipe sediment data and include it in a run. The pipe sediment data will then override values in the sediment depth field. If the depth of the passive layer is equal to or greater than the maximum sediment depth, there will be no sediment in the active layer.

Ackers White Model

This section describes the Ackers White algorithms available for calculating the erosion and deposition of sediment in pipes. The algorithm is based on the Ackers-White theory (Ackers and White, 1973).

The erosion and deposition calculations are made at the end of every water quality timestep after the advection equations have been solved. The algorithm is as follows:

1. At each computational point along each pipe, a non-dimensional carrying capacity (C_v) is calculated that represents the maximum concentration of a given sediment fraction that can be held within the flow. The equation used to calculate C_v is written:

Equation 3-23

$$C_v = J\left(\frac{W_e R}{A}\right)^{\alpha}\left(\frac{d_{50}}{R}\right)^{\beta}\partial_c^{\gamma}\left\{\frac{u}{\sqrt{g(s-1)R}} - K\partial_c^{\delta}\left(\frac{d_{50}}{R}\right)^{\varepsilon}\right\}^{m}$$

Where:

C_v = non-dimensional carrying capacity (-)

W_e = the effective bed width (m)

R = hydraulic radius of flow (m)

A = cross sectional area of the flow (m^2)

d_{50} = average sediment particle size (m)

u = flow velocity (m/s)

g = acceleration due to gravity (m/s^2)

s = specific gravity of sediment particles (-)

∂_c = the composite friction factor, calculated using the Colebrook-White formula as described in Voogt, van Rijn and van den Berg, (1991)

$J, \alpha, \beta, \delta,\ K,\ \gamma,\ \varepsilon,\ m,$ = coefficients dependent on the dimensionless grain size D_{gr}.

Equation 3-24

$$D_{gr} = d_{50}\left(\frac{g(s-1)}{\mu^2}\right)^{\frac{1}{3}}$$

Where:

D_{gr} = grain size (-)

d_{50} = the average sediment particle size (m)

μ = the kinematic viscosity of water (m^2/s)

g = the acceleration due to gravity (m/s^2)

s = the specific gravity of the sediment fraction (-).

2. The non-dimensional carrying capacity number is converted to a maximum concentration by:

Equation 3-25

$$C_{max} = C_v \rho s$$

Where:

C_{max} = maximum carrying concentration (kg/m^3)

C_v = non-dimensional carrying capacity (-)

ρ = density of fluid (kg/m^3)

s = the specific gravity of the sediment fraction (-).

3. If the actual concentration is greater than C_{max} then the excess sediment is deposited. If the actual concentration is less than C_{max} the bed is eroded until either C_{max} = C_{actual} or all the bed has been eroded. Erosion is assumed to occur instantaneously while the rate of deposition is a function of the sediment settling velocity.
4. All flow concentrations and bed masses are updated before the sediment is advected at the next timestep.

The Ackers White model has been utilised throughout this study; thus, full description has been provided, alternatively, the Velikanov and Zug Model can be used to calculate erosion and deposition in pipes. The Velikanov model determines two concentrations (C_{min} and C_{max}). If the flow concentration is below C_{min} then erosion occurs to achieve C_{min} if possible. If the flow concentration is above C_{max} then deposition occurs to achieve C_{max} if possible. If the flow concentration is between C_{min} and C_{max} then no erosion or deposition occurs. The KUL model was developed at the Katholieke Universiteit Leuven in Belgium, the model determines two shear critical stress values (*tau* critical deposition and *tau* critical erosion). If the shear stress is below *tau* critical deposition, then deposition occurs. If the shear stress is above *tau* critical erosion, then erosion occurs. If the shear stress is between *tau* critical deposition and *tau* critical erosion, then no erosion or deposition occurs. The rate of deposition or erosion depends on shear stress. All erosion and deposition calculations are made at the end of every water quality timestep after the advection equations have been solved.

The four catchment models as represented in the InfoWorks CS software are presented in Figure 3-3, Figure 3-4, Figure 3-5 and, Figure 3-6, the CSO spill data used in this study was collected in CSO conduits highlighted in red, these spill pipes can be seen to correspond with the CSO's in Figure 3-2.

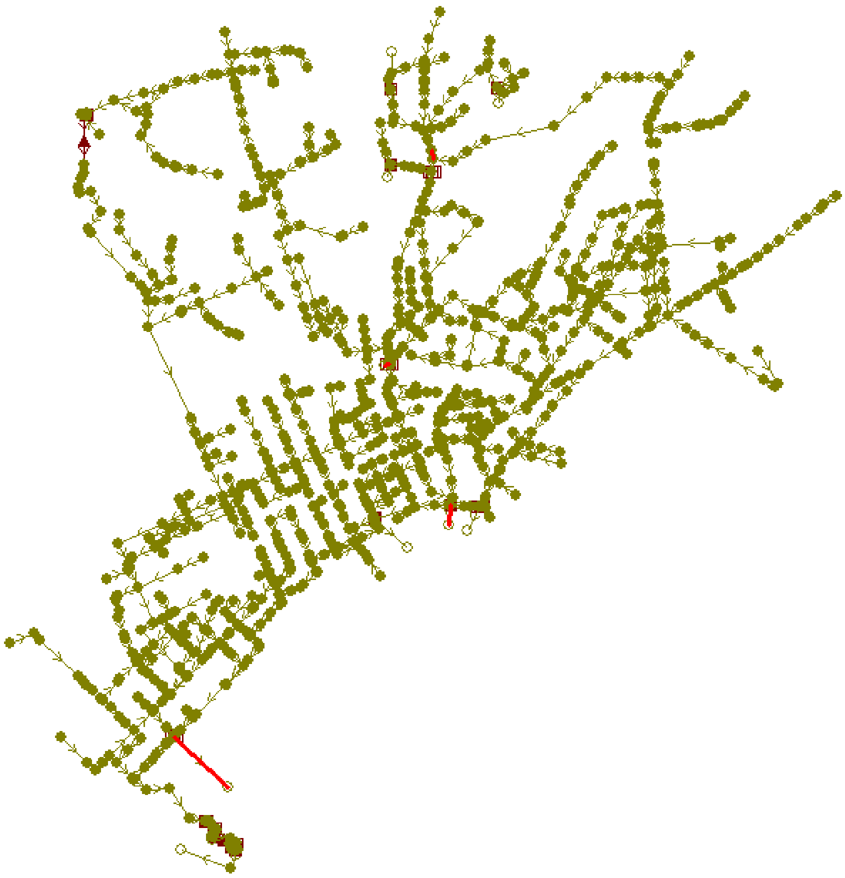

Figure 3-3 Ashton-Under-Lyne InfoWorks CS sewer network model (Catchment A) – CSO spill pipes monitored 3, 4, 5 and 7 are highlighted in red

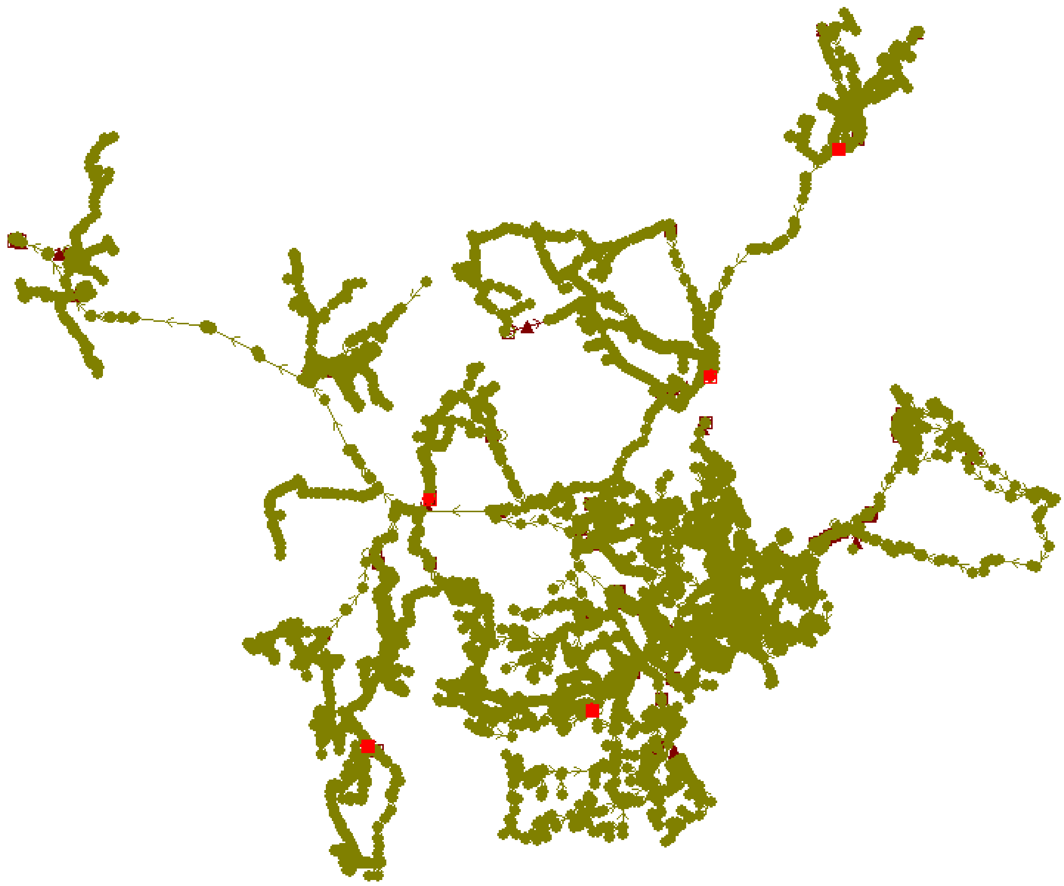

Figure 3-4 Dukinfield InfoWorks CS sewer network model (Catchment B) – CSO spill pipes monitored 1, 2, 6, 8 and 9 are highlighted in red.

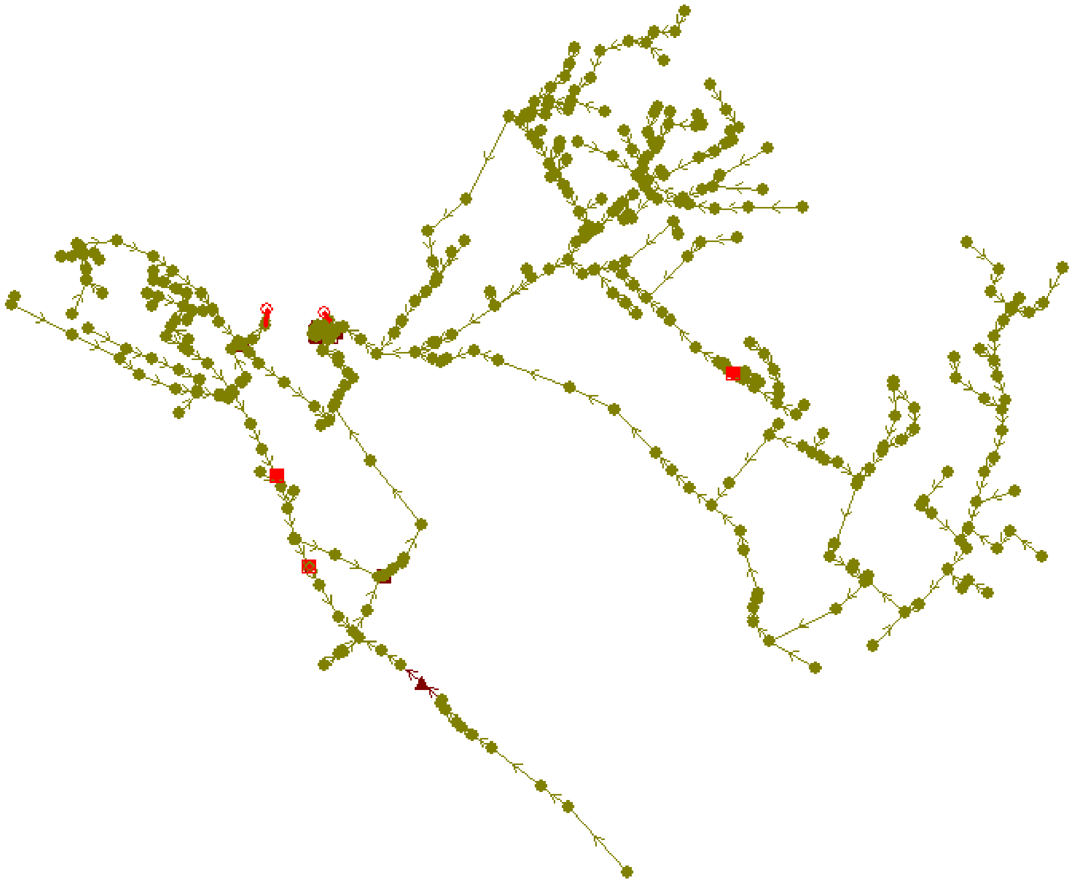

Figure 3-5 Hyde InfoWorks CS sewer network model (Catchment B) – CSO spill pipes monitored 10, 11, 12, 13 and 14 are highlighted in red.

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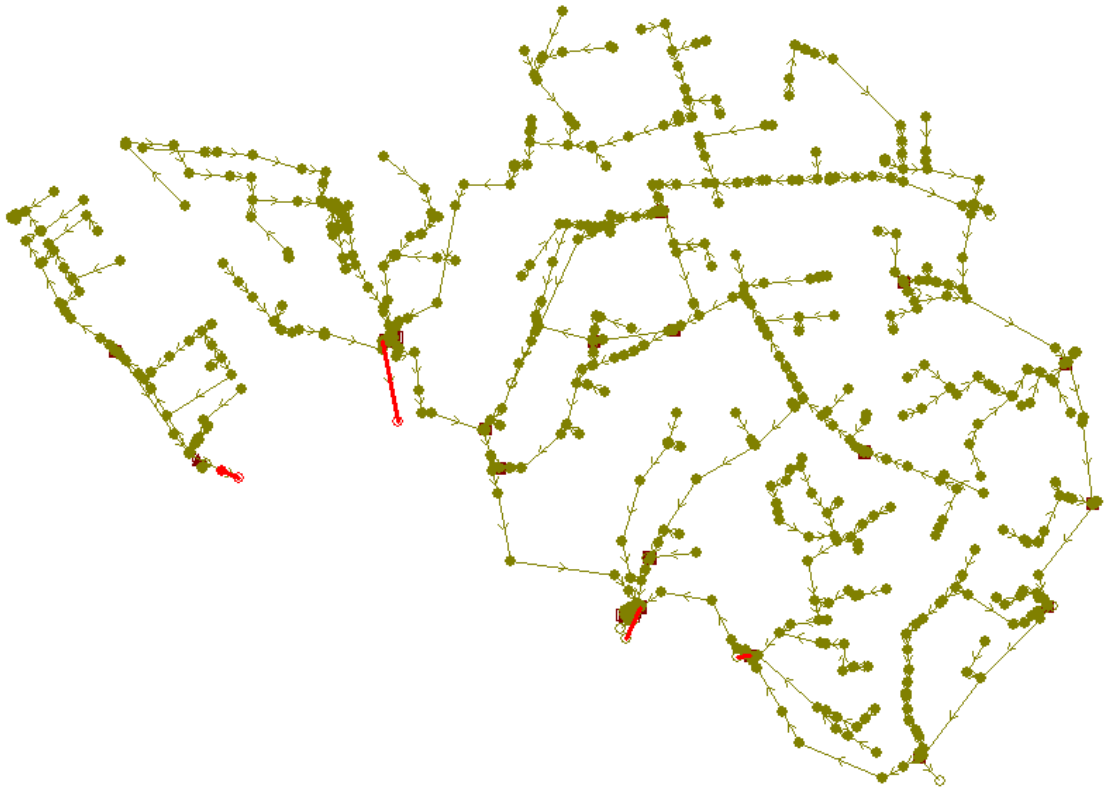

Figure 3-6 Denton InfoWorks CS sewer network model (Catchment D) – CSO spill pipes monitored 15, 16, 17 and 18 are highlighted in red.

3.2.3 River Model

The DUFLOW model was used to model the river Tame in the integrated model (IHE Delft, 1995). It is a network model in which the rivers and their main tributaries are represented by a network of branches and nodes. The branches represent individual stream sections while the nodes represent confluences, bifurcations, inflow locations or other locations where model results are required.

The DUFLOW model is a computer package for simulating one-dimensional unsteady flow, it utilises the 1D Advection Diffusion Equation to describe the concentration of quality parameters as a function of time and space. The hydraulic model within DUFLOW can be directly coupled with one of two pre-defined water-quality models EUTROF1 and EUTROF2. EUTROF1 model is a predefined eutrophication model which describes the cycling and transformation of water quality parameters without considering interaction between the water column and channel sediment. It is based on the EUTRO4 model from WASP4 developed by the U.S. EPA (Ambrose et al. 1988). For the TAME Integrated catchment modelling study, EUTROF1, was used to simulate water quality in the river systems within the river Tame. Water quality constituents that can be simulated in EUTROF1 are dissolved oxygen (DO), biochemical oxygen demand (BOD), algal biomass, components of the nitrogen cycle (organic nitrogen, ammonia, nitrate), components of the phosphorous cycle (organic and inorganic phosphorous), and suspended solids. Only BOD, COD and TSS water quality variables were simulated in this study. A schematic representation of the river Tame represented in the DUFLOW model is shown in Figure 3-7.

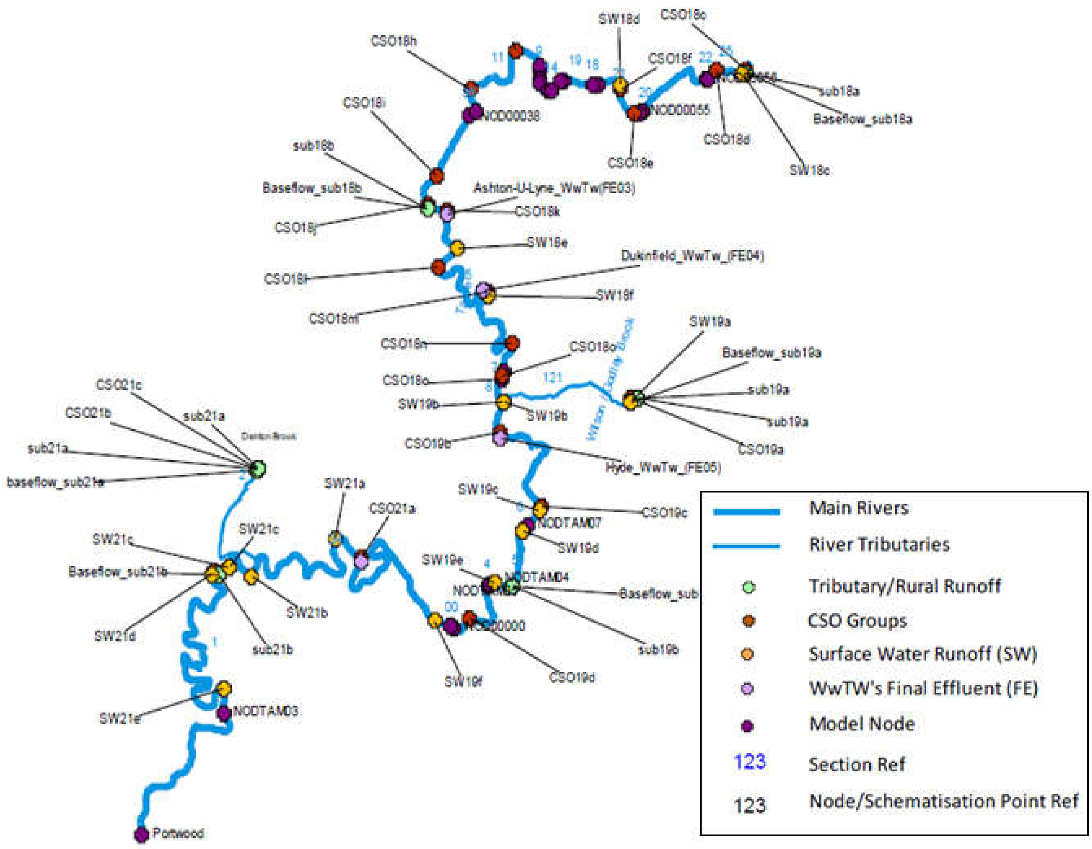

Figure 3-7 River TAME and respective inputs represented in DUFLOW modelling software

3.2.4 Water Quality Monitoring

To assess the impact of the 18 CSO's highlighted by the EA as 'unsatisfactory' on the River Tame, water quality monitoring campaign was conducted over a period of two months within the catchment. The monitoring campaign was carried out by consultant contractors Montgomery-Watson-Herza (MWH) in conjunction with the EA. MWH were selected from the United Utilities approved contractors list; a list of contractors whose work meets the necessary criteria to be classified as adhering to 'best industry practice' by Unities Utilities and the EA. Whilst information on the monitoring campaigns structure is presented, due to the monitoring campaign being carried before this study, limited detailed information regarding the sampling methodology is available, however, it is assumed that due to the campaign being carried out under the authority of the EA, all 'best practice' sampling procedures in conjunction with those expressed in the WaPUG (1998a) guidelines have been adhered to; location of samplers, transportation of samples, laboratory testing and statistical analysis. Subsequently, it is assumed that the resulting data generated from the monitoring campaign is of sufficient accuracy to be used in this study.

Water quality loggers were placed in the continuation pipes of the 'unsatisfactory' CSO's within each sewer catchment and at 6 in-river locations previously highlighted as 'sensitive' to intermittent discharges by the EA (Figure 3-8). Further to this, in order to confirm the sensitivity of the river to intermittent discharges, the dynamic pollutant descriptions of BOD and NH_4 river model inputs (InfoWorks CS outputs for rainfall event 2) were replaced with EMC's in the typical range expected from that of extremely dilute sewage to crude sewage (Table 3-3).

Table 3-3 ***EMC input concentration for river sensitivity analysis***

	EMC Sewer model output	
Model Input Reference Number	BOD (mg/l)	NH_4 (mg/l)
1	8.75	1.1
2	17.5	2.3
3	35.4	4.6
4	70.9	9.3
5	140	18.7
6	280	37.5
7	560	75

Figure 3-8 shows the river models response to the 8 EMC inputs and the observed values recorded at river monitoring location 2, it was determined that the river was sensitive to intermittent discharges at all six of the locations highlighted by the EA, thus it is hypothesised that any changes to the description of water quality outputs from the sewer model (CSO spill event description) for use as inputs to the river model, would be reflected in the modelled concentrations at these locations.

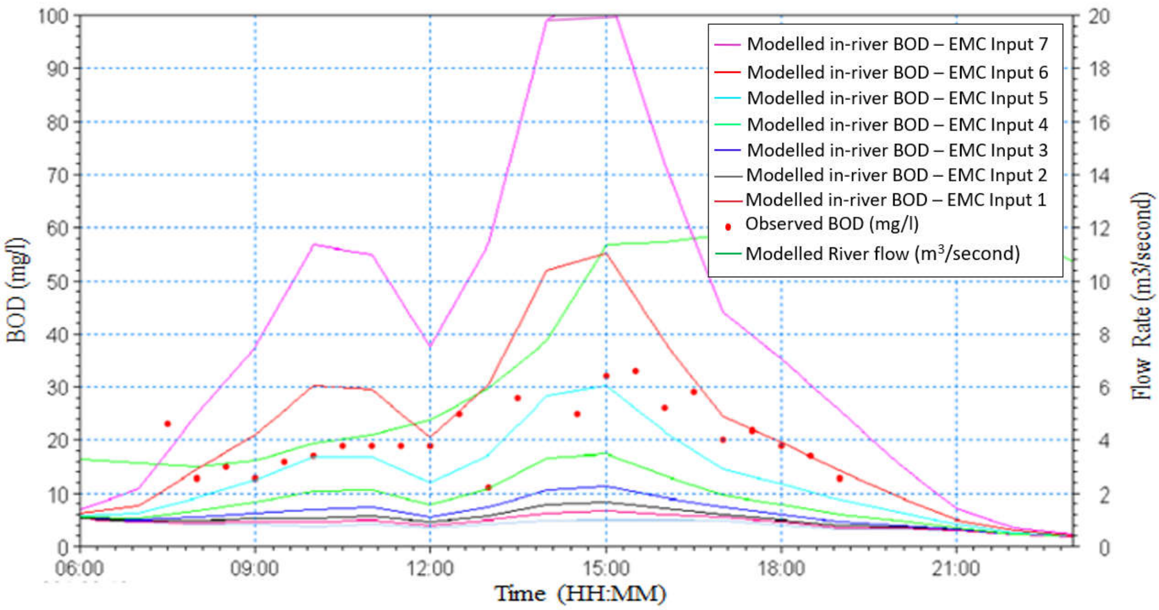

Figure 3-8 River model response to varying EMC inputs and observed BOD at river monitoring station 2.

Data Collection

Loggers were remotely triggered to take samples of intermittent discharges during spill events. Water quality measurements following two rainfall events are presented in this work. During each rainfall event a different number of spills were recorded at each CSO. The data collection exercise captured time series concentration data of BOD, NH_4 and TSS every 15 minutes during each event. Time series rainfall data (recorded in mm every 2 minutes for the duration of each rainfall event) was collected via tipping bucket rain gauges (see Figure 3-2 for location). Rain gauge data was used as inputs to each sub-catchment's hydraulic sewer model, which was then run to determine the start/end time, volume and duration of CSO spills within the study. Table 3-4 presents sub-catchment averaged rainfall characteristics for the two rainfall events.

Table 3-4 ***Summary characteristics of rainfall event***

Sub-Catchment	Average Intensity (mm/hr)		Peak intensity (mm/hr)		Depth (mm)		Duration (hrs)	
	Rainfall Event		Rainfall Event		Rainfall Event		Rainfall Event	
	1	2	1	2	1	2	1	2
A	1.2	2.9	42.8	10.5	19.4	7.4	15.8	2.5
B	1.5	2.3	11.3	7.8	15.9	5.8	10.5	2.5
C	1.1	2.0	17.7	5.4	23.3	2.2	21.4	1.1
D	1.1	2.9	13.2	12.0	30.3	6.4	2.5	2.2

3.2 Analysis: Calculation of EMCs and Variance for each Spill Event

For the two rainfall events with corresponding water quality data, a total of 29 independent spill events were recorded at monitored CSOs within the catchment. Mean concentrations of BOD, NH_4 and TSS were calculated over each of the spill events recorded by the water quality loggers; this was defined as the 'optimum' EMC for each spill event. The difference between the optimum EMC value and the actual concentration parameter entering the receiving water will vary over each spill event due to the temporal variability of the rainfall event and pollutant transport processes. For each event (*i*) of length (*n)* the mean variation $V_{E,}$ between the optimum EMC and the measured data (BOD, NH_4 and TSS) for each spill event is defined as:

Equation 3-26

$$V_E = \sqrt{\sum_{t=0}^{t=n} \left(M_{i,t} - EMC_i\right)^2}$$

Where:

V_E = mean variation between the EMC for event i and the measured data for each event i (mg/l)

$M_{i,t}$ = the measured parameter during spill event i at time *t* (mg/l)

EMC_i = EMC for the spill event i (mg/l).

To identify the relative scale of this variance it is directly compared to the variation between predictions using the pre-calibrated InfoWorks CS sewer model used within the ICM study and the measured data for each spill event. This mean variance, V_i for each event (i) is defined as:

Equation 3-27

$$V_i = \sqrt{\sum_{t=0}^{t=n} \left(M_{i,t} - P_{i,t}\right)^2}$$

Where:

V_i = Minimum achievable variance between observed and predicted quality parameters for each event (mg/l)

P_{it} = the predicted value of the concentration parameter during event *I* at time *t* (mg/l)

$M_{i,t}$ = the measured parameter during spill event i at time *t* (mg/l).

An example of the variance analysis is presented in Figure 3-9.

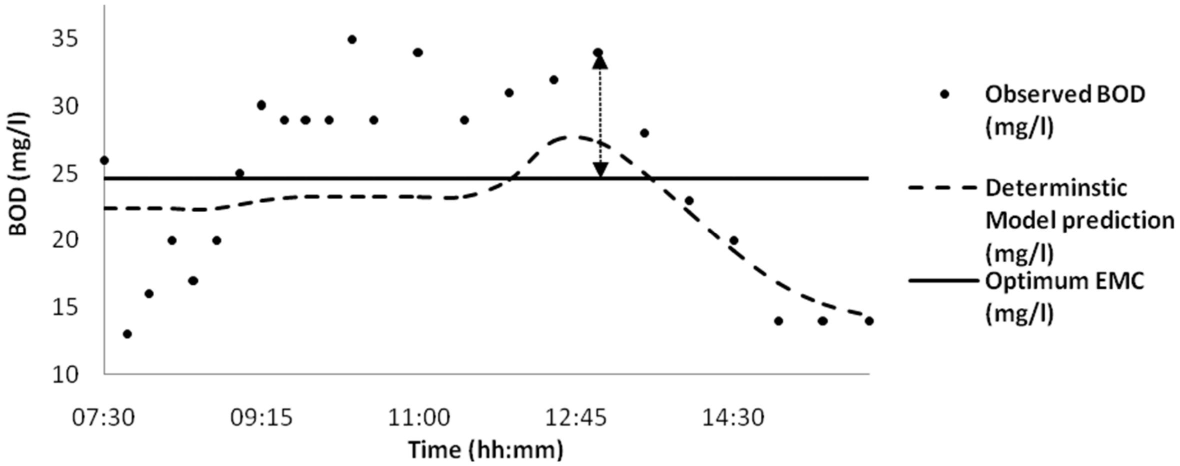

Figure 3-9 BOD measured spill event with calculated optimum EMC and prediction using calibrated InfoWorks CS/ICM model. Recorded spill details: date 16/01/2012, spill time 07:30 – 15:05, catchment D, rainfall event 1, CSO 16.

In the original ICM river impact study carried out by United Utilities, InfoWorks CS predictions of spill concentrations were used as inputs to the river impact model. To assess the relative significance of using mean concentrations within an ICM study, these InfoWorks CS predictions were replaced with optimum EMC values (for monitored CSOs) and sub-catchment event mean concentrations (for unmonitored CSOs), all other input parameters were unaltered. For both the original ICM study and the mean concentration methodology the variance between the modelled and observed water quality parameters at the six water quality sampling locations was quantified using Equation 3-27 for each spill event. An example of this analysis is presented in Figure 3-10.

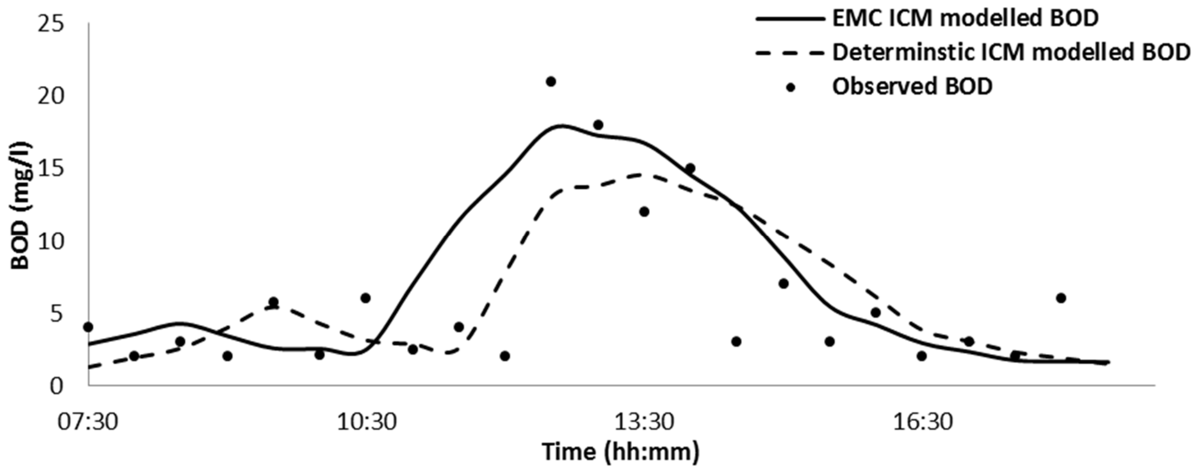

Figure 3-10 BOD measured within receiving waters after a spill event compared with associated ICM predictions using both mean concentration

and InfoWorks CS. Recorded spill details: date 16/01/2012, time 07:30 - 18:31, catchment C, rainfall event 1, CSO 12.

3.3 Results

3.3.1 Sewer Quality Results

Tables 3-4, 3-5 and 3-6 show the calculated optimum EMCs as well as mean variances, V_E and V_i calculated using Equation 3-26 and Equation 3-27 for each monitored CSO spill event.

Table 3-5 Characteristics of each spill event and measured variances for BOD

Sub-catchment	Rainfall Event	CSO	Spill Duration (hh:mm)	Optimum EMC	Deterministic Variance (V_i)	EMC Variance, (V_E)
				BOD (mg/l)	BOD (mg/l)	BOD (mg/l)
A	1	7	00:50	25.3	34.4	4.0
A	1	4	04:00	23.4	16.6	7.3
A	1	3	03:25	23.2	23.0	10.5
A	1	5	05:00	41.2	15.4	11.2
B	1	2	06:46	33.5	87.4	12.5
B	1	1	07:30	62.3	167.9	14.7
B	1	9	00:42	13.0	11.6	0.7
B	1	8	20:39	51.9	13.4	9.7
B	1	6	01:32	90.3	46.0	18.1
C	1	10	00:52	20.0	8.1	21.0

C	1	13	12:14	5.3	75.5	7.7
C	1	12	11:01	8.5	8.0	0.7
C	1	14	02:01	112.5	33.2	14.0
C	1	11	04:26	83.9	83.0	5.6
D	1	15	05:55	30.3	13.1	14.1
D	1	16	07:35	24.6	4.9	6.3
D	1	17	01:55	30.4	10.6	29.9
A	2	7	04:05	37.5	7.4	40.7
A	2	3	01:50	45.0	90.6	52.8
A	2	5	01:30	101.4	49.1	48.1
B	2	2	01:27	124.8	3.9	43.7
B	2	1	01:28	142.5	5.5	40.6
B	2	6	00:41	100.7	1.4	51.5
C	2	14	01:22	139.0	116.2	8.5
C	2	11	02:45	133.0	86.8	35.2
D	2	15	00:51	152.7	89.1	58.2
D	2	17	00:50	151.0	201.6	82.4

Table 3-6 Characteristics of each spill event and measured variances for NH_4

Sub-catchment	Rainfall Event	CSO	Spill Duration (hh:mm)	Optimum EMC	Deterministic Variance, (V_i)	EMC Variance, (V_E)
				NH_4 (mg/l)	NH_4 (mg/l)	NH_4 (mg/l)
A	1	7	00:50	3.7	1.7	1.1
A	1	4	04:00	4.2	2.1	1.4
A	1	3	03:25	2.7	2.1	1.1
A	1	5	05:00	4.6	1.4	1.6
B	1	2	06:46	1.6	8.1	0.9
B	1	1	07:30	5.5	6.0	2.0
B	1	9	00:42	1.9	0.5	0.7
B	1	8	20:39	7.5	3.9	1.5
B	1	6	01:32	2.2	0.4	0.6
C	1	10	00:52	0.9	0.1	0.4
C	1	13	12:14	0.5	3.5	0.5
C	1	12	00:29	0.9	0.5	0.3
C	1	14	02:01	28.8	3.0	4.1
C	1	11	04:26	9.4	1.6	2.7
D	1	15	05:55	2.7	0.8	1.1
D	1	16	13:35	7.2	3.2	2.3
D	1	17	01:55	2.8	1.0	1.2

A	2	7	04:05	6.4	1.1	4.6
A	2	3	01:50	15.2	3.2	2.4
A	2	5	01:30	14.0	4.9	9.7
B	2	2	01:27	15.5	0.7	0.1
B	2	1	01:28	20.8	0.8	5.3
B	2	6	00:41	8.0	0.3	1.2
C	2	14	01:22	15.6	10.2	3.0
C	2	11	02:45	8.6	3.3	1.6
D	2	15	00:51	11.1	5.2	2.2
D	2	17	00:50	14.0	10.2	7.1

Table 3-7 Characteristics of each spill event and measured variances for TSS

Sub-catchment	Rainfall Event	CSO	Spill Duration (hh:mm)	Optimum EMC	Deterministic Variance, (V_i)	EMC Variance, (V_E)
				TSS (mg/l)	TSS (mg/l)	TSS (mg/l)
A	1	7	00:50	34.6	32.3	6.4
A	1	4	04:00	41.7	19.1	9.4
A	1	3	03:25	26.9	29	7.4
A	1	5	05:00	48.2	18.3	13.4
B	1	2	06:46	50.4	44.1	14.6
B	1	1	07:30	72.1	101.2	14.7

B	1	9	00:42	19	8.4	3.6
B	1	8	20:39	84.1	14.6	12.4
B	1	6	01:32	103.6	33.3	23.4
C	1	10	00:52	42.3	9	26.7
C	1	13	12:14	11.2	67	11.7
C	1	12	00:29	14.6	9.2	2.6
C	1	14	02:01	162.3	27.4	16.7
C	1	11	04:26	74.1	79.6	7.4
D	1	15	03:36	30.4	10.2	11.3
D	1	16	13:35	44.6	4.2	8.4
D	1	17	01:55	40.1	11.4	36.5
A	2	7	04:05	50.3	11.6	42.1
A	2	3	01:50	62.3	74.6	59.3
A	2	5	01:30	144.2	44.2	44.8
B	2	2	01:27	163.3	6.2	42.6
B	2	1	01:28	174.1	7.4	36.7
B	2	6	00:41	114.3	2.4	53.5
C	2	14	01:22	140.3	105.7	7.4
C	2	11	02:45	144.3	77.6	34.2
D	2	15	00:51	141.3	93.4	62.4
D	2	17	00:50	172.1	178.6	77.4

During event 1, mean optimum EMC's of 40.0mg/l, 5.1mg/l and 52.9 mg/l were observed for BOD, NH_4 and TSS respectively. Significantly higher mean EMC's of 112.8mg/l, 12.9mg/l and 130.6 mg/l were observed during event 2. The average variance between optimum EMC's and observed values (V_E) across all events FOR BOD was 24.1 mg/l, compared to a variance of 48.3mg/l using the deterministic model (V_i). The average variance between optimum EMC's and observed values (V_E) across all events for NH_4 was 2.9 mg/l, compared to a variance of 2.2 mg/l using the deterministic model (V_i). The average variance between optimum EMC's and observed values (V_E) across all events for TSS was 41.4 mg/l, compared to a variance of 25.4 mg/l using the deterministic model (V_i).

Minimum EMC Variance and Rainfall Characteristics

It is hypothesized that the minimum EMC variance is linked to the nature of the rainfall event which caused hydraulic overload of the drainage system. As shorter, more intense rainfall events are more temporally and spatially variable, such events may cause spills with a greater degree of temporal variation than longer more 'steady' events. Representation of these events using a mean value may therefore cause a higher degree of inherent variance between predicted and observed spill characteristics.

Figures 3-11 and 3-12 show the variance between BOD measured and Optimum EMC and NH_4 measured and optimum EMC versus the average intensity of the rainfall event that caused the associated CSO spill respectively.

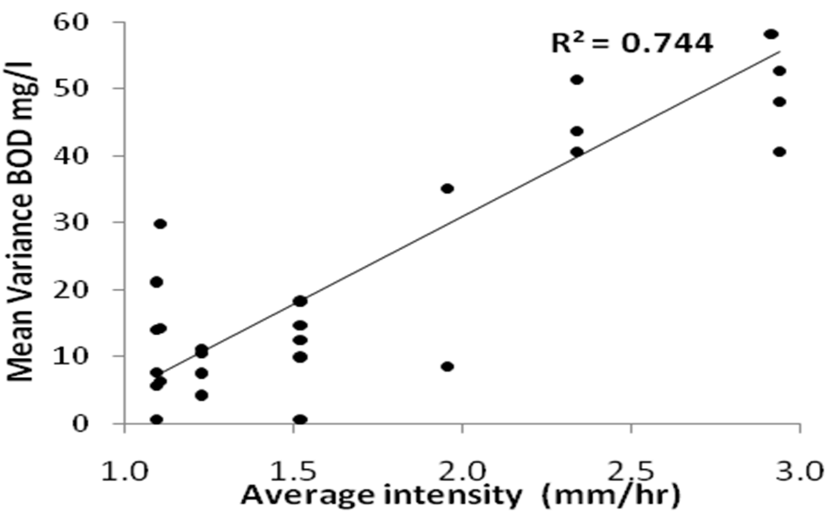

Figure 3-11 Minimum variance of EMC (V_E) for BOD versus average intensity of all rainfall events for all measured data presented in Table 3-5.

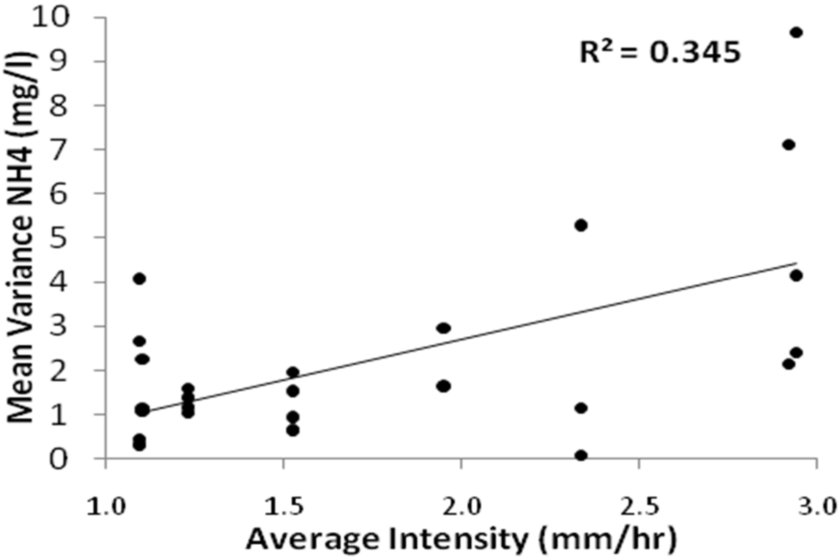

Figure 3-12 Minimum variance of EMC (V_E) for NH_4 versus average intensity of all rainfall events for all measured data presented in Table 3-6.

A positive correlation can be seen between the intensity of rainfall events and variance between EMC's for BOD. The trend for NH_4 is less clear.

3.3.2 River Quality Results

Tables 3-7, 3-8 and 3-9 present the variance between observed and model predicted water quality parameters at each 'in river' water quality monitoring location. The 'deterministic' variance represents the variance between observed water quality parameters and the DUFLOW model utilising InfoWorks CS dynamic pollutant descriptions as inputs. The 'Mean' variance represents the variance between observed water quality parameters and the DUFLOW model predictions utilising the optimum EMC values presented in section 3.3. Optimum EMC values were used in conjunction with hydraulic flows calculated by InfoWorks CS for all spills.

Table 3-8 In-river variances between observed BOD measurements and those predicted by the DUFLOW model using InfoWorks CS (deterministic) and optimum EMC values for CSO spills.

River Monitoring Location/Station	Event 1		Event 2	
	Deterministic Input Variance	Mean Input Variance	Deterministic Input Variance	Mean Input Variance
	BOD (mg/l)	BOD (mg/l)	BOD (mg/l)	BOD (mg/l)
1	12.3	11.9	1.5	1.7
2	13.5	9.9	3.3	2.8
3	15.9	52.3	4.8	3.6
4	9.6	6.7	3.1	3.9
5	3.2	3.3	5.1	13.8
6	7.9	6.7	2.7	4.1
Average Variance	10.4	15.1	3.4	5.0

Table 3-9 In-river variances between observed NH_4 measurements and those predicted by the DUFLOW model using InfoWorks CS (deterministic) and optimum EMC values for CSO spills.

River Monitoring Location/Station	Event 1		Event 2	
	Deterministic Input Variance	Mean Input Variance	Deterministic Input Variance	Mean Input Variance
	NH_4 (mg/l)	NH_4 (mg/l)	NH_4 (mg/l)	NH_4 (mg/l)
1	0.12	0.15	0.13	0.13

2	0.63	0.68	0.49	0.65
3	0.72	0.70	0.75	0.79
4	0.52	0.58	0.61	0.88
5	0.50	0.44	0.60	1.31
6	0.43	0.48	4.05	0.71
Average Variance	0.49	0.51	1.11	0.75

Table 3-10 In-river variances between observed TSS measurements and those predicted by the DUFLOW model using InfoWorks CS (deterministic) and optimum EMC values for CSO spills.

River Monitoring Location/Station	Event 1		Event 2	
	Deterministic Input Variance	Mean Input Variance	Deterministic Input Variance	Mean Input Variance
	TSS (mg/l)	TSS (mg/l)	TSS (mg/l)	TSS (mg/l)
1	20.4	16.8	2.4	2.21
2	18.4	14.1	5.7	4.7
3	21.3	55.7	7.4	6.7
4	14	14.2	3.4	24.4
5	6.5	6.8	8.9	18.7
6	12.9	9.4	4.5	5.4
Average Variance	15.58	19.50	5.38	10.35

3.4 Discussion and Conclusions

In this chapter, the use of a hydrodynamic deterministic sewer model to describe CSO spill events resulted in predictions with a greater mean predictive variance when compared to optimum EMC's derived from observed data. Whilst the 'optimum' EMC methodology presented here is not a predictive technique, the results indicate there is significant potential to use EMC's to describe CSO spills as an alternative to deterministic models if accurate methods for EMC prediction are used. Whilst optimum EMC's vary significantly across different sub-catchments, no notable relationship between EMC's or deterministic model variances and catchment characteristics were observed.

Analysis of storm events suggests that the potential accuracy of EMC's is linked to properties of rainfall events; shorter duration, high intensity events being inherently more variable with time. This trend is more evident for BOD and TSS than NH_4, it cannot be said with certainty, but this could be linked to the portions of total TSS and BOD which are derived from the catchment surface, as NH_4 is more commonly associated with wastewater flows (Brombach, et al, 2005). It is known that storm water TSS concentration values are inherently linked to a rainfall events ability to mobilise particles on the catchment surface (Brodie & Roswell, 2006), thus an increased intensity could cause increased variation of TSS values around that of a mean representative value for a given spill event. Large fluctuations of TSS around a representative mean value could also be linked to a phenomenon described as the 'first flush', whereby significantly large portions of total TSS and BOD loads in a given spill event are witnessed at the beginning of a storm event (Bach *et al.,* 2010a). It is recognized that a more detailed analysis and further datasets are required to adequately explore the relationship between the temporal and spatial variation of rainfall events and water quality characteristics of spill events.

Analysis of the river quality datasets show that for this catchment the variance between the observed and predicted water quality parameters is of a similar scale when both the mean concentrations and deterministic models are used to describe the CSO spill events. It is apparent that the observed predictive variance is higher during the more intense rainfall event. In nearly all six river locations the difference in variance between both methods is relatively small when compared to the actual observed variance; this would suggest that for this catchment the most significant source of variance between the ICM methodology and observed values is derived from the river impact model itself, and that the different methods of pollutant description (dynamic and EMC) are of less significance. This could be either due to model structure or that the adopted calibration procedure is not robust. This would also suggest that there is significant potential to use simpler mean concentrations within ICM's as there would appear to be no significant loss of accuracy in final receiving water quality predictions.

Chapter 1 introduced the concept of intermittent urban discharges; chapter 2 gave an overview of the Integrated Catchment Modelling framework ultimately highlighting how the use of simple water quality description techniques could aid the application of the ICM process. The chapter related the variance between EMC and 'dynamic' observed values to rainfall characteristics and shows that these variances, whilst noticeable, may not be significant in contrast to observed variances when using industry standard deterministic sewer and river water quality models. Hence it is evaluated that there is significant potential for more widespread use of EMCs within integrated modelling approaches if a 'reliable' EMC prediction methods can be found.

Research groups have previously developed and successfully verified the use of EMC models on catchments where they were originally formulated (Dembélé *et al.,* 2011); however, with water quality data often limited, the transferability of these models to catchment other than where they were developed is limited within the literature (Dotto, 2010). Whilst this chapter showed the potential for the use of the EMC pollutant description technique within the ICM approach, in order to further understand this potential and with the key aim of this thesis being to develop a new simplified modelling technique, the underlying science behind simple EMC models and their transferability to new catchments needs investigation, chapter 4 seeks to address this need.

Chapter 4. Evaluating the performance of EMC models using case study data

The aim of this chapter is to robustly test a previously published EMC methodology presented within the literature to evaluate the transferability of this ‘simple’ approach to water quality modelling, and to subsequently provide recommendations to aid the development of a new novel EMC water quality model in chapter 5. A version of this chapter was presented at the 10th International Urban Drainage Modelling Conference (Norris et al., 2015).

With the overarching aim of this work being to ‘develop’ a new novel water quality model, the UK water quality data set presented in chapter 3 was deemed unsuitable for model development due to an insufficient number of water quality events available for study (Fletcher and Deletic 2008). For this reason, a new comprehensive TSS storm water quality data set provided by Monash University has been presented in this chapter. For this reason, at this point in the thesis, the scope of the work is narrowed to the development of a novel TSS EMC storm water model, thus an in-depth description of the key processes affecting variations in TSS storm water quality; build-up and wash-off, and further literature on the development of simple storm water TSS EMC modelling techniques has been presented. Due to data gathering limitations, BOD and COD models have not been investigated further in this work.

4.1 Background to storm water modelling of total suspended solids

A number of research groups have suggested that suspended solids are the most appropriate indicator of urban runoff pollution levels within stormwater flows, It has been suggested that many other problematic pollutants become attached to the finer fractions of TSS, thus when evaluating urban runoff pollution, the prediction of TSS concentrations or loads is considered the most important requirement for any storm water model (Deletic, 1997). As an alternative to ‘complex’ deterministic quality models, several research groups have developed simple regression-based models to predict TSS Event Mean Concentrations (EMC) based on catchment type and rainfall event characteristics. Whilst the use of such models to estimate TSS pollutant concentrations has been achieved with mixed success, this success is inherently sensitive to the strength of available experimental data that can be used for calibration (Dembélé *et al.,* 2010). It is generally agreed that land use has an important impact on TSS concentrations, however establishing any explicit relationships which allow transferability of default model parameter values across catchments has been achieved with little success (Maniquiz et al., 2010). Mitchell 2001 presented average values of storm water TSS EMC's and specific TSS EMC values associated with various land use types, these values are presented in Table 4-1 and Table 4-2 respectively.

Table 4-1 Average Storm water TSS EMC values recorded in urban areas (adapted from Mitchell 2001)

	Mitchell (2001)	Duncan (1999)	US EPA (1983)	US EPA (1999)	Ellis (1989)	Williamson (1991)
TSS EMC (mg/l)	138.9	154	174	78.4	190	170

Table 4-2 Storm water TSS EMC values for given land uses (adapted from Mitchell 2001)

	Land Use Category	Mean	1st Quartile	3rd Quartile
TSS EMC (mg/l)	Urban Open	126	57	280
	Developed	77	32	190
	Urban Roads	191	101	361

The values show that TSS EMC's can vary significantly across catchments and between different areas of land use, section 4.1 presents information within the literature concerning the processes that influence these variations.

4.2.1 Stormwater Processes influencing TSS pollutant concentrations

This section looks further into the literature in an attempt to further understand the processes which cause variations in TSS concentrations; four key processes influence these variations (Murphy, Cochrane and O'Sullivan, 2015):

- Atmospheric deposition of pollutants on the catchment surface.
- Build-up of pollutants on the catchment surface.
- Wash-off of pollutants on the catchment surface.
- Transportation of pollutants washed off within the UDS.

Whilst the atmospheric deposition and build-up of pollutants are explicitly independent processes, in the context of study, they are difficult to separate due to the quantity of pollutant build-up being directly influenced by atmospheric deposition (Egodawatta, Ziyath and Goonetilleke, 2013). It is also considered very difficult to explicitly separate the wash of pollutants from the catchment surface and their transportation to receiving water bodies; this is due to the spatial resolution of monitoring campaign water quality loggers, normally located at the downstream discharge point of catchments under study (Bertrand-Krajewski, Chebbo and Saget, 1998). For the remainder of this work, the first two processes; Atmospheric deposition and build-up of pollutants, and the latter two processes; wash-off and transportation of pollutants are described together as 'build-up' and 'wash-off' respectively.

Pollutant Build-Up

Sartor (1974) presented significant work into the build-up of pollutants by studying their behavior on various types of urban street surfaces. The study suggested that pollutant build up is greater in industrial areas due to the poor condition of vehicular surfaces and in areas of road sweeping, it was the first study to also present the link between pollutants and the finer fraction of solids in build-up material. The relationship between antecedent dry weather periods (ADWP) defined as the time period preceding the rainfall event/wash off event under analysis) and pollutant build-up is still not clear; however, it is assumed and accepted that build-up is a function of ADWP (Deletic, Maksimovic and Ivetic, 1997).

Modelling descriptions of the pollutant build-up process generally focus on the processes of pollutant accumulation following a rainfall event and the deposition of materials from traffic, via wind and numerous other sources (Deletic, Maksimovic and Ivetic, 1997). Grottker (1987) suggested that material is deposited at an increased rate during the first 24 hours following a rainfall event, whilst many authors have agreed with this hypothesis, due to the variations and lack of confidence in results, no specific technique has been agreed to describe pollutant build-up. It has been suggested that the two processes; Atmospheric deposition of pollutants on the catchment surface and the build-up of pollutants on the catchment surface reach a state of equilibrium after approximately 9 days (Pal, Wallis and Arthur, 2011).

Descriptions of pollutant accumulation used in build-up models vary significantly; linear, exponential and constant relationships have all been used to describe the relationship between accumulated pollutant load on the urban surface and a rainfall events preceding ADWP. In the most basic sense, these descriptions assume that the pollutant load accumulated starts at zero after a rainfall event; they thus lack the ability to account for accumulation of loads and cases where the entire pollutant load is not removed from the urban surface during the previous rainfall event. Ball et al., (1998) suggested that power functions were the most reliable mathematical description of pollutant build-up, however, Sartor and Boyds original description of pollutant build-up still remains the most common descriptor used in modelling practice. Table 4-3 shows some of the typical mathematical equations used to model pollutant build-up within the literature.

Table 4-3 Pollutant build-up equations

Equation	Definition	References
$y = a + \frac{b}{x}$	x = Antecedent dry period (days)	(Ball, Jenks and Aubourg, 1998)
$y = a + b \ln x$ $y = ae^{-bx}$	y = Accumulated pollutant (g/m^2)	(Egodawatta, Thomas and Goonetilleke, 2007)
$y = \min(c, ax^b)$	$a, b,$ and c = Calibration parameters	(Chow, Yusop and Abustan, 2015)

Whilst no mathematical description of pollutant build-up has been universally agreed within the literature, it is acknowledged that build-up does not infinitely increase with ADWP and at some point in time following a rainfall event, the amount of pollutant load available to be washed off increases no further (Deletic, Maksimovic and Ivetic, 1997). It has been suggested that pollutants initially accumulate at a high rate and that the rate of accumulation is followed by a decreased accumulation rate and asymptotes to a threshold level (Goonetilleke, Egodawatta and Kitchen, 2009). Hatt *et al.*, (2004) suggested that the rate of increase is specific to each individual catchment. In many build-up models, such as the stormwater management model (SWMM), the user is offered a choice of different build-up functions (US EPA). Vaze et al., (2003) concluded that the amount of pollutant surface load does not automatically translate to the amount of pollutant washed off the urban surface, and that the proportion of pollutant washed off is significantly influenced by other factors.

Vaze et al., (2003) investigated the type of material which accumulates on urban surfaces, they suggested that two different types of particle make up the surface load; free and fixed. The work suggested that free loads (loads made up of particles 'easily' removable) decrease after a rainfall event and that the consistency between daily accumulation levels was low. It was also suggested that total build up, even of the free load particle category is not reduced to zero following a rainfall event. This work suggested that a rainfall event of sufficiently high intensity would be necessary to provide enough energy for both types of particles to be completely removed. The work further proposed that these 'free' types of particle were replaced quite easily by the movement of particles in wind and deposition from vehicular sources. The MOSQITO model was developed based around this theory; separating accumulated fractions into varying cohesive strengths, however its application is limited due its extra step of complexity and lack of proven increased performance when compared to models that do not include this particle cohesive theory (Crobeddu and Bennis, 2011).

Pollutant Wash-off

The removal and transportation of accumulated pollutants into stormwater runoff is known as wash-off. Two main physical processes govern the variations in pollutant wash-off loads and concentrations; the removal of particulates from the urban surface due to rainfall drops impact energy and the removal of particulates via shear stress provided by overland flow (Egodawatta, Thomas and Goonetilleke, 2007).

Numerous researchers have highlighted the significance of rainfall characteristics on pollutant wash-off (Brodie and Rosewell, 2007; Egodawatta, Thomas and Goonetilleke, 2007). It has been suggested that increases in wash-off TSS concentrations are related to the intensity of the rainfall event in which the wash-off occurred (Brodie and Dunn, 2010). It is widely accepted that the more intense a rainfall event, the more energy can be supplied on impact to the accumulated layers of pollutant, thus allowing greater quantities of wash-off to become mobilised and entrained within stormwater flow (Van Dijk et al., 2002). Two commonly used equations presented by Sartor and Boyd (1974) and Egodawatta et al., (2007) to describe pollutant wash-off respectively are:

Equation 4-1

$$W_t = W_0(1 - e^{-KIt})$$

Where:

W_t = transported sediment load after time t (g/m^2)

W_0 = Initial load of material on surface (g/m^2)

K = Calibration parameter (mm^{-1})

I = Rainfall Intensity (mm/hr)

t = time (hr).

and:

Equation 4-2

$$F_W = \frac{W}{W_0} = C_f(1 - e^{-KIt)}$$

Where:

F_w = Fraction of wash-off (-)

W = Weight of material mobilized (g/m^2)

W_0 = Initial mass of material on surface (g/m^2)

C_f = Capacity factor (-)

K = Calibration parameter (mm^{-1})

I = Rainfall Intensity (mm/hr)

t = time (hr).

Egodawatta et al., (2007) suggested that the amount of pollutant washed off is related to the intensity of rainfall and the accumulated pollutants characteristics. Brodie and Rosewell (2007) suggested that the kinetic energy provided by raindrops is a dominant guiding process in the prediction of pollutant wash-off. Studies on catchment in the United States by Jewell and Adrian (1982) suggested that when trying to link various rainfall and catchment characteristics to event loads and fluxes, not one set of variables was found to consistently outperform another, indicating that not one set of catchment or rainfall variables is better at predicting pollutant wash-off.

Deletic et al., 1997 used Ordinary Least Squares (OLS) regression and achieved R-squared values of 0.65 when comparing observed TSS loads with predicted values by creating a model which included particle detachment from raindrop energy and total shear stress. Irish et al., 1998 built upon this work, adapting the method to predict highway runoff, the work suggested that TSS is affected more by ADWP than other pollutants.

A 'first-flush' is a term used to describe a phenomenon when significantly large portions of the total pollutant load derived from a rainfall event are temporally distributed in the early phases of the rainfall event under analysis (Bertrand-Krajewski et al., 1998). The presence and definition of this phenomenon argued by various authors with some studies failing to confirm its existence (Deletic 1998).

4.2.2 Simple Approaches to Stormwater TSS modelling

Due to the stochastic nature and inter-process variability of build-up and wash-off processes, building models that can accurately and consistently predict storm water quality remains a difficult task. Many authors have citied that the problem be so site specific and stochastic in nature, that no one technique can be 'best' for every modelling problem, subsequently, a large number of mathematical techniques with varying degrees of complexity are available to storm water quality modellers (Zhang *et al.*, 2015). In line with a key philosophy often associated with modelling problems, Franciscan friar William of Ockham suggested that when two competing theories make the same prediction, the simpler one is the most appropriate (Sorensen, 2011). In line with this paradigm and considering the conclusions of chapter 3, a review of 'simple' methodologies capable of producing Event Mean Concentrations of TSS has been presented in this section.

Event based EMC models are statistical models which can be used to describe the generation of pollutants. The models describe pollutants in terms of loads or concentrations, which can then be multiplied by the discharging/event volume of a system or catchment to determine total event loads (Charbeneau and Barrett, 1998). The use of purely statistical EMC modelling approach has generally been accepted as a tool suitable for longer term impact assessment (Charbeneau and Barrett, 1998) the wider implementation of this approach is hindered by the significant variation in EMC concentrations across urban catchments, even those with similar land and hydrological characteristics (Chiew and McMahon, 1999). In further detail, whilst these simple model functions may adequately describe build-up and wash-off processes, catchment specific calibration of parameter values is necessary, subsequently, collection of calibration data sets can incur significant further costs during the calibration procedure (Dotto *et al.*, 2011). Whilst physically descriptive complex models have larger numbers of parameters that need calibrating due to the many different processes represented in these models, in contrast, simple models require more temporarily distributed data, but for the calibration of fewer parameters (Kleidorfer *et al.*, 2009).

Probabilistic EMC models such as MUSIC are often more sophisticated models that stochastically generate EMC's concentrations based on predefined pollutant distributions, these models ignore build up and wash off processes, ultimately predicting event loads concentrations by deriving statistical relationships between observed values and catchment characteristics (Dotto *et al.*, 2011). A move from simply statistical EMC techniques towards EMC techniques which have some method of physical description has seen the development of conceptual-empirical regression-based EMC models. During the 1980's, a national stormwater quality monitoring study in France allowed for the examination of statistical relationships between TSS and storm characteristic variables. In the two urban catchments under study, maximum rainfall intensity was used to successfully describe the variance in EMC TSS values; R^2 values of approximately 0.9 and 0.6 were reported (Desbordes and Servat, 1983). The study concluded that when using maximum rainfall intensity and runoff volume as variables, errors of 30% and 10% were calculated for individual event EMC's and annual totals respectively.

In the United States, the Nationwide Urban Runoff Program (US EPA, 1983) measured urban runoff water quality in 28 urban catchments. Driver and Tasker (1988) and used regression analysis to conclude that rainfall duration and maximum rainfall intensity were the most important variables to explain the variance in TSS EMC's. The event variable ADWP has been implemented to improve these regression models in urban catchments (Driver and Troutman, 1989).

In Australia, a review of urban stormwater processes by Duncan (1995) incorporated the wash-off potential energy of rainfall events into a simple power equation to predict event loads, Vaze and Chiew (2003) used regression analysis to examine the use of various rainfall characteristic within this model in comparison with a widely used deterministically process based model (SWMM) (Huber and Dickinson 1998), the work suggested that when using rainfall intensity as a variable within the power equation, the predictive capabilities of both the simple calibrated power equation and the process model were similar.

Dotto *et al.*, (2010) examined the performance of three empirical continuous concentration models widely adopted in practise; STORM (USACE, 1977), SWMM (Rossman, 2010) and P8-UCM (Palmstrom & Walker, 1990). This work suggested that whilst models which used 'routed' variables were more accurate than those which did not, the temporal accuracy gained by this extra step of complexity was not likely to outweigh the extra calibration costs, furthermore, it argued that to develop efficient pollution generation models, future research efforts should be directed toward the use of models which use explanatory factors such as ADWP and rainfall event variables.

The literature reviewed showed that in the context of storm water quality, accounting for build-up and wash-off processes appears fundamental when trying to predict variations in TSS concentrations, and that rainfall event characteristics, in particular, the variable rainfall intensity is a key driver in TSS pollutant generation due to the role it plays in the wash-off process. It is therefore hypothesized that any description of stormwater TSS should account for both build-up and wash-off processes; by utilizing a conceptual relationship between TSS EMC’s and some form of rainfall event characteristic. The literature also showed that storm water models have been developed which accurately predict catchment EMC’s, their application remains limited to the catchments in which they were developed, thus their transferability to new catchments remains unknown. To address this unknown, the remainder of this chapter uses case study data to evaluate the transferability of the EMC model presented in Dembélé *et al.,* (2011) to catchments other than where it was originally developed.

4.3 Transferability of EMC TSS storm water quality models

The key objective of this work was to develop a novel water quality model, one which could improve the application of the integrated modelling methodology, in turn helping water utilities reduce the negative impact of urban discharges. To develop a model with the aforementioned characteristics, a data set containing catchment storm water outfall TSS water quality measurements and respective rainfall event characteristics was required. Whilst monitoring campaigns designed to provide data for model development have been deployed at various spatial and temporal resolutions, in accordance with (Leecaster, Schiff and Tiefenthaler, 2002), it was determined that the UK water quality data set used in chapter 3 (data collected for 5 WQ events over four different catchments) was not adequate for model development. In respect of this issue and the thesis objectives, following oral presentation of the work described in chapter 3, a comprehensive water quality data set was obtained courtesy of a research placement with Professor Ana Deletic at the Water Sensitive Urban Design group at Monash University.

Dembélé et al. (2011) published an empirical model capable of predicting stormwater EMC TSS, the model linked catchment TSS EMC’s to explanatory rainfall characteristics; rainfall depth (DURA) and ADWP. The model was derived and calibrated for two catchments in Lyon, France: Chassieu and Ecully (Table 4-4). Calibration and verification of this model was judged to be a success; mean values of calibration uncertainties less than 20%, low variabilities in model parameters and model verification efficiency coefficients of approximately 0.5 (J.

E. Nash and Sutcliffe, 1970). The calibration and verification of the model was only conducted using 21 events on two catchments, thus to assess the transferability of this model, it has been applied to new comprehensive water quality dataset.

Table 4-4 Characteristics of catchments used in Dembélé et al., (2011)

Site	Primary Land Use	Area (ha)	Total Impervious Fraction
Ecully	Residential	245	0.42
Chassieu	Industrial	185	0.75

The extensive high-resolution water quality data set was obtained courtesy of Monash University. The Monash monitoring program was performed to take representative samples of urban runoff during storm water events across several catchments with varying land use characteristics. The program was unique to previous large-scale monitoring studies in that it measured very short-term rainfall intervals with accompanying water quality data. A total of 237 rainfall events and corresponding storm water quality data were monitored across 6 urban catchments in Melbourne Australia (Table 4-5). Further to the information presented in this thesis, details of the monitoring campaign can be found in Mitchell *et al.*, (2008).

Table 4-5 Catchment characteristics and number of events monitored for each catchment.

Catchment Reference	Primary Land Use	Area (ha)	Total Impervious Fraction	No. of events monitored
GR	Industrial	28.2	0.8	60
RICH	High Density Residential	89.1	0.74	54

RCW	Medium Density Residential	105.7	0.51	34
SHEP	Medium Density Residential	38	0.45	20
NW	Low Density	10.5	0.2	55
ER	Mixed residential and commercial	186	0.46	22

The following section provides information regarding the original monitoring program and preliminary data analysis. It should be noted that further to the receipt of the raw data (excluding the definition of rainfall event start and end times) all data analysis was carried out independent to those presented in McCarthy *et al.*, (2008); Mitchell *et al.*, (2008) and Dotto *et al.*, (2011).

4.4 Overview of Monitoring Campaign

Rainfall was measured using onsite tipping buckets with measurement volumes of 0.2mm at a temporal resolution of 1 minute; these were positioned as near to the centroid of each catchment as possible. Flow rates were recorded by Sigma 900 auto-samplers located in the respective storm water collection systems pipe outlet, flow rates were measured every 1 minute. After each rainfall event, monitors were inspected and cleaned to ensure water quality sampling was carried out effectively. Discrete pollutant sampling was carried out for Total Suspended Solids (TSS), Total nitrogen (TN), Total Phosphorus (TP) and E.coli. TSS water quality data and respective rainfall event data are utilized in this work. Wet weather samples were collected via autosampler connected to a flowmeter at each catchment respectively; the samplers were triggered to sample after a 'significant' increase in flow was detected by the flow meter (McCarthy *et al.*, 2008). The samplers were programmed to sample for a 1 in 3 month return period event, this period of time was estimated using the MUSIC software package developed at Monash University (CRCCH 2003). The following sampling regime presented in Fletcher and Deletic (2008) was adhered to:

- Of 24 bottles, the first 10 were sampled uniformly to account for the initial 30% of flow volume;
- 10 bottles were used for the next 40% of flow volume; and
- the Remaining 4 bottles for the last 30% of the event.

The method was refined during the sampling period once expected volumes respective to each catchment were established. The specific regime was adopted as a trade-off between good capture of rising limb pollutant concentrations and the total capture of large events.

The land use of each catchment was established according to Melbourne's Department of Sustainability and Environment planning scheme zonings classifications (Melbourne's Department of Sustainability and Environment, 2005). The impervious fraction of each catchment was established via the use of aerial orthophotos and site inspection. This information was used to create an area based weighted average to estimate the total fraction of impervious area. One-meter topographic contours were utilized to estimate the average slope of all catchments. To ensure that 'actual' rainfall events were recorded, average run-off coefficients (total runoff volume divided by rainfall depth multiplied by area) were calculated for each catchment, if extreme values were recorded (those significantly greater than 1), these data were excluded from the data set.

For an event to start, over 0.2mm of rainfall needed to be recorded at the tipping gauge. An event was finished if no rainfall was detected for four hours. The ADWP for each rainfall event was defined as the total time in days between the previous and selected rainfall event, ADWP was extracted straight from continuous daily rainfall records recorded by Melbourne Water, these records were provided by Monash University. The data were synthesized in preparation for model calibration of the model presented in Dembélé *et al.,* (2011); for each event, total suspended solids event mean concentration (TSS EMC), antecedent dry weather period (ADWP) and rainfall duration (DURA) were defined as follows;

- Total Suspended Solids event mean concentration (TSS EMC) (mg/l); mathematically defined as the average of the TSS samples recorded between the specified event start and end time.
- Antecedent dry weather period (ADWP) (days); extracted from continuous rainfall records, the time between the previous and selected rainfall event.

- Rainfall Duration (DURA) (mins); the total time between the commencement and last recorded tip of the respective catchment rainguage.
- Rainfall Depth (DEPT) (mm); sum of all recorded tips during from the first recorded and last recorded tip throughout the duration of the selected rainfall event.
- Average rainfall intensity (AGI5) (mm/hr); division of total rainfall depth by the rainfall duration.
- Initial average ten-minute rainfall intensity (IT10) (mm/hr); Initial average rainfall intensity recorded from the first ten-minute period of each rainfall event.

The variables DURA and AGI5 were not required for testing of the model but are later utilised in chapter 5; for simplicity, they have presented in section 4.4.1.

4.4.1 Univariate Analysis of Monitoring Campaign Data

Univariate analysis was performed on all variables to provide understanding of the data. The parameters Mean ($\tilde{x}$), standard deviation (SD) and coefficient of variation (CV) were selected to describe the given data sets. The mean of a given data set is its most representative single value, calculated using Equation 4-3:

Equation 4-3

$$\tilde{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$$

Where:

for each observation x_i,

$\tilde{x}$ = the mean of the observed variable (mg/l)

n = the number of observations in the data set.

The standard deviation (SD) of a given data set is a single value which represents the dispersion of data points around the mean. The more concentrated a given data set is around the mean, the smaller the SD value will be. The SD was calculated using Equation 4-4:

Equation 4-4

$$SD = \sum_{i=1}^{n} \sqrt{\frac{(x_i - \tilde{x})^2}{n}}$$

Where for each observation x_i,

SD = standard deviation (mg/l)

$\tilde{x}$ = the mean of the observed variable (mg/l)

n = the number of observations in the data set.

A summary of the univariate statistics derived for each catchments TSS EMC's is presented in Table 4-6, corresponding quartile box plots of catchment TSS EMC's are shown in Figure 4-1 and the respective quartile statistics used to create these box plots in Table 4-7.

Table 4-6 Summary of catchment TSS EMC's

		Catchments						
Catchments		ER	GR	NW	RCW	RICH	SHEP	Mean
TSS EMC (mg/l)	Mean	60.8	59	99	78	97	62	76
	SD (mg/l)	56.5	40.4	72.8	74.1	82.9	61.9	64.8

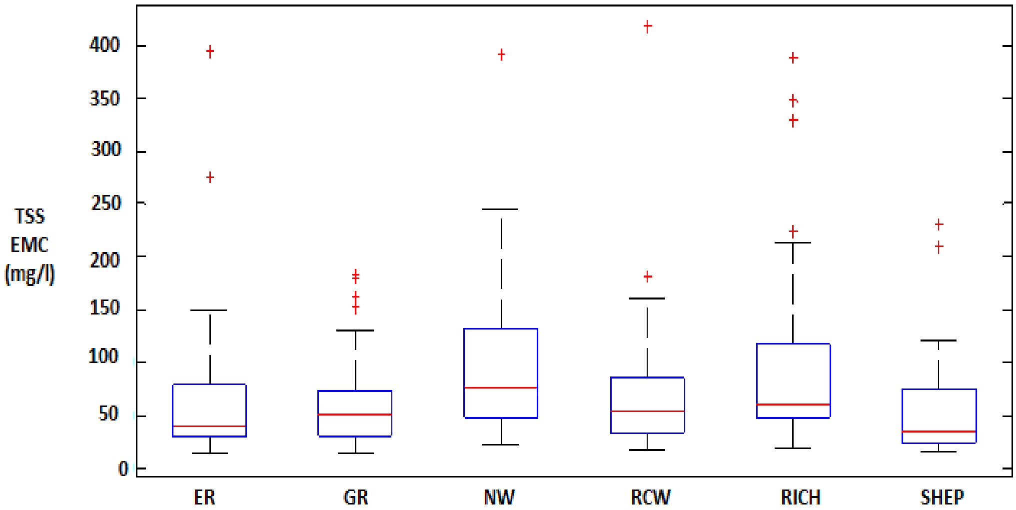

Figure 4-1 Box plots of catchment TSS EMC's

Table 4-7 Box plot statistics of catchment TSS EMC's

	ER	GR	NW	RCW	RICH	SHEP
Upper (mg/l)	149.3	130.7	244	161.7	213	119.7
75th Percentile (mg/l)	79.3	73.9	131.8	85	117.7	74.7
Median (mg/l)	40.4	50.9	76.1	53.4	59.6	34.4
25th Percentile (mg/l)	29.3	31.2	47.8	33.4	48.6	23.94
Minimum (mg/l)	13.4	13.3	21.9	17.7	19.5	16.7
Maximum (mg/l)	393.8	183.1	392	418.5	388.6	230

Table 4-6 shows the mean and standard deviation of TSS EMC's for each respective catchment. Whilst the mean across all catchment seems relatively stable, in the range (59-99 mg/l), Figure 4-1 and Table 4-7 show that event EMC's vary significantly with minimum and maximum EMC values recorded during certain rainfall events of 13.3 and 418.5 mg/l respectively, SD values of 40.4 to 82.9 confirm this observation. These large variations in EMC's show the potential need for some physical/process description when attempting to predict EMC's, and the dangers of using simple site mean concentration models that are based on recorded values of EMC's alone.

In the context of catchment land use characteristics, the RICH and NW catchments showed the largest variations (SD values) in TSS EMC's; 82.91 and 72.8 mg/l respectively. Both the NW and RICH catchments are residential areas, comparing SD values from these catchments to those observed in the industrial catchment GR; 40.4 mg/l, it could suggest that large variations in TSS EMC's could be linked to the inherent uncertainty more commonly associated with human behaviours which influence pollutant build-up (traffic patterns, construction activities). Conversely, 'medium density residential' catchments showed low variance of TSS EMC's around each catchment's respective mean, thus is it concluded that in this study, the results of the water quality monitoring campaign would suggest that it is difficult to describe variations in TSS EMC's with respect to land use characteristics. A summary of respective rainfall event statistics for each catchment is presented in Table 4-8.

Table 4-8 Summary of univariate statistics for catchment rainfall events

	Statistic	ER	GR	NW	RCW	RICH	SHEP	Mean
No Events	-	24	60	55	34	54	20	-
Antecedent Dry Weather Period (Days)	Mean	2.9	3.13	3.05	2.28	2.64	3.15	2.9
	Range	0.64-7.25	0.09-23.06	0.1-46.0	0.08-16.8	0.40-28.2	0.50-13.3	-
	SD	2.0	4.3	7	3.7	4.5	3.3	4.1

	CV	0.71	1.37	2.31	1.64	1.29	1.10	1.40
Rainfall Duration (mins)	Mean	374	285	324	349	281	425	339
	Range	56-1351	16-987	140-1256	12-1326	14-1012	18-1409	-
	SD	288	209	300	294	238	400	288
	CV	0.77	0.97	0.93	0.85	0.83	0.94	0.88
Rainfall Depth (mm)	Mean	9.29	7.43	10.11	6.58	7.33	10.1	8.5
	Range	1 – 23.4	0.8 – 38.6	0.2 – 33.1	0.6 – 20.8	0.80-39.2	0.6-35.4	-
	SD	7.8	6.1	7.8	4.9	6.8	24	9.6
	CV	0.84	0.82	0.78	0.78	0.93	1.61	0.96
Average Rainfall Intensity (mm/hr)	Mean	2.1	2.5	3.2	2.2	3.6	3.1	2.6
	Range	0.5–12.5	0.4-30.1	0.29-19.9	0.1-16	0.4-28	0.5-13.3	-
	SD	2.4	6.1	7.8	3.9	4.2	3.5	4.8
	CV (%)	1.17	0.82	0.78	0.78	1.59	1.10	1.04

Table 4-7, shows statistical information on the rainfall events responsible for TSS EMC's. The largest SD values of the variable ADWP were associated with the rainfall events recorded on the RICH and NW catchments; 4.5 and 7 days respectively. Furthermore, the variable 'rainfall intensity' associated with RICH and NW had the largest mean and largest variation; mean intensity of 3.6 and 3.2 mm/hr, with SD's of 4.2 and 7.8 mm/hr respectively. Whilst it is difficult to draw any specific conclusions regarding this univariate analysis, these initial results tend toward the hypothesis that the TSS EMC values recorded during this monitoring campaign are driven by rainfall characteristics rather than land use characteristics. The variable driving variations in TSS EMC are considered further in chapter 5.

Huber (1986), Duncan (1999) and Francey *et al.*, (2004) suggested that catchment storm water TSS EMC event data follows a log-normal distribution; the Lilliefors test was used to test this hypothesis on the Melbourne data set within the software package Matlab version R2013a (www.mathworks.com). The Lilliefors test applies a test decision for the null hypothesis that the data comes from a distribution in the normal family (thus the data was first transformed), against the alternative that it does not; rejected at the 5% significance level. Following transformation of EMC TSS concentrations for all catchments, each catchments data set met the null hypothesis (Table 4-9), confirming a non-normal distribution.

Table 4-9 Lilliefors test statistics applied to Melbourne catchment EMC data

Catchment EMC's	Null Hypothesis 1 = Reject	P-Value	KSTAT	Critical Value
ER	0	0.50	0.10	0.15
GR	0	0.50	0.06	0.11
NW	0	0.50	0.07	0.12
RCW	0	0.36	0.11	0.15

RICH	0	0.04	0.13	0.13
SHEP	0	0.06	0.19	0.19

Catchments event TSS EMC's were sorted in ascending order and fitted with an exponential trend line, 'closeness of fit' to this trend (indicated by the OLS 'closeness of fit' indicator R^2), Figure 4-2 presents all derived catchment TSS EMC's.

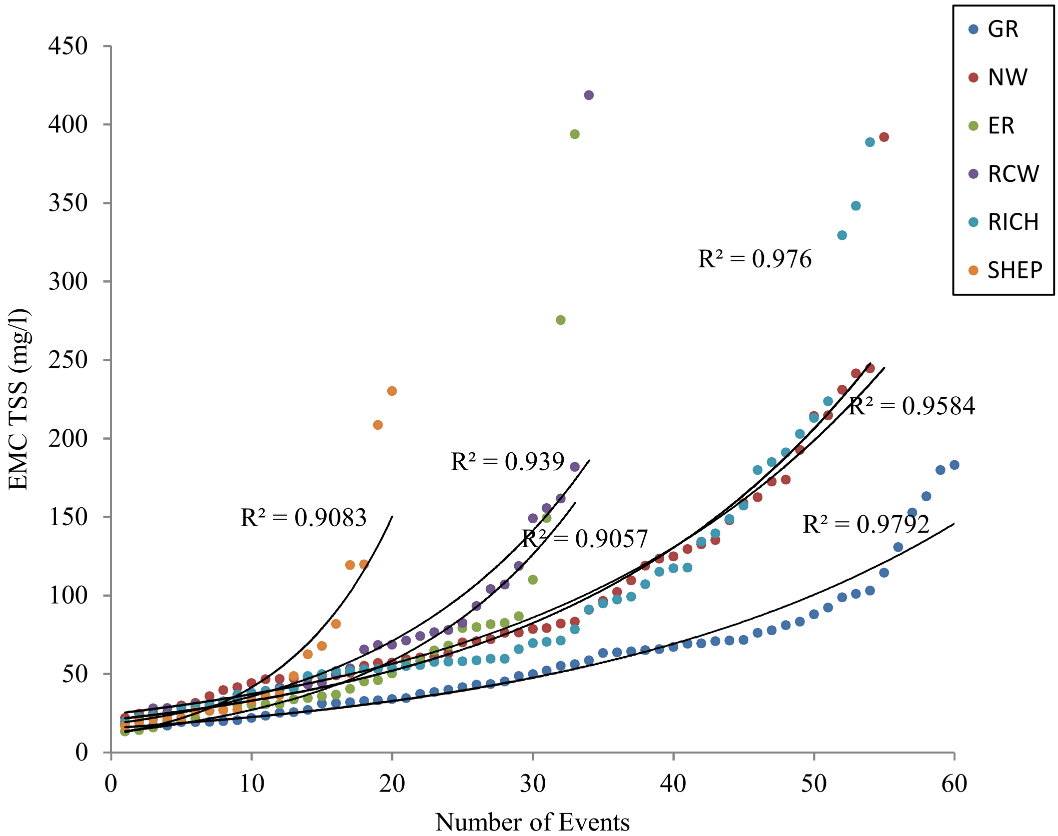

Figure 4-2 Event TSS EMC's sorted in ascending order and plotted for each catchment, R^2 value shows least squares closeness of fit to exponential trend line.

4.5 Calibration of TSS EMC model

The TSS EMC model presented in Dembélé et al. (2011) describes two distinct behaviours during a rainfall event; in the first part, the model assumes a logarithmic increase of TSS EMCs, with rainfall depth which becoming the limiting factor, defined by a threshold value λ. In the second declining part, TSS EMCs decrease with the rainfall depth as the accumulated mass is the limiting factor (Equation 4-3).

Equation 4-5

$$\frac{dEMC}{dX} = \frac{b_1}{X}(X \leq \lambda) + \frac{b_3}{X^2}(X > \lambda)$$

Where:

EMC = TSS EMC (mg/l)

X = Rainfall Depth (mm) * Antecedent dry weather period (days)

λ = threshold value of X separating the two behaviors of EMC values

b_1 and b_3 = model calibration parameters (-).

The final equation of the model is obtained by analytical integration of Equation 4-5:

Equation 4-6

$$EMC = [(b_1 \ln(X) + b_2)(X \leq \lambda)] + \left[\left(\frac{b_3}{X} + b_4\right)(X > \lambda)\right]$$

Where:

EMC = TSS EMC (mg/l)

X = Rainfall Depth (mm) * Antecedent dry weather period (days)

λ = the threshold value of X separating the two behaviors of EMC values

b_1, b_2, b_4 and b_3 = model calibration parameters (-).

Calibration of the model is carried out in two steps, firstly a specific algorithm is applied to calculate the value of λ, and secondly, the Levenberg-Marquardt algorithm (damped least-squares fitting minimisation technique used to solve non-linear least squares problems) was used to estimate b_1, b_2, b_3 and b_4. Further information on model formulation both the specific calibration and Levenberg-Marquardt algorithm is described in Dembélé et al. (2011). The observed data sets for each catchment were used to calibrate and validate each catchment, data were split randomly 80:20 for calibration and validation respectively (Figure 4-3 and Figure 4-4 respectively).

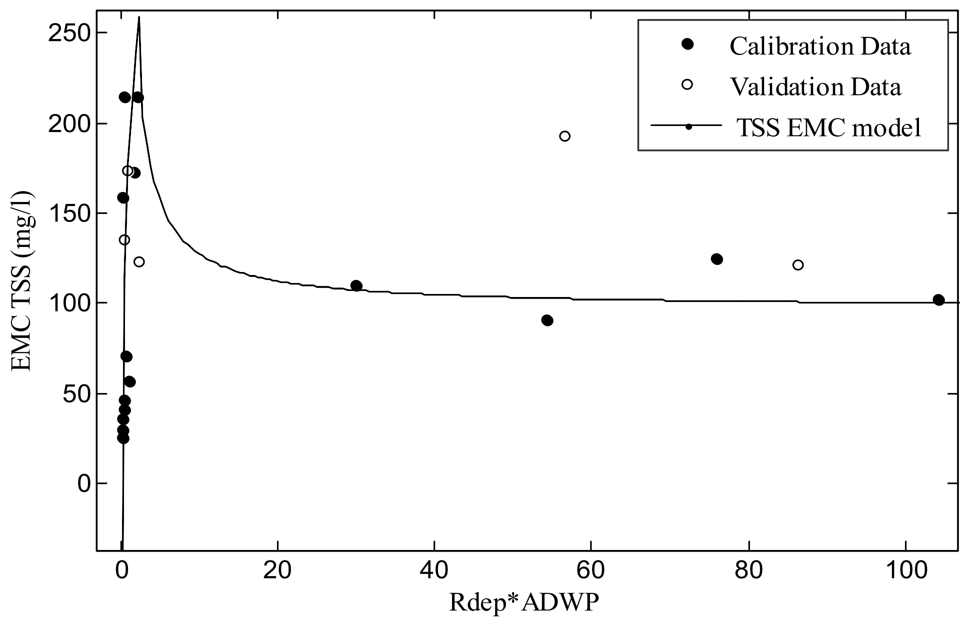

Figure 4-3 Observed data used for calibration of model and validation in NW catchment.

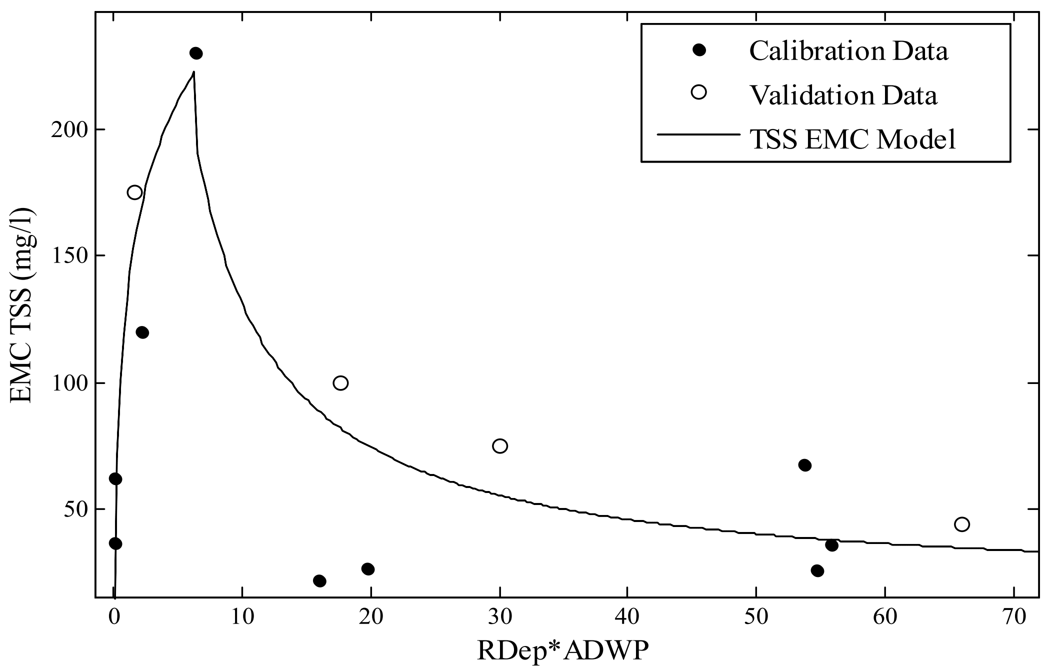

Figure 4-4 Observed data used for calibration of model and validation in SHEP catchment.

4.6 Discussion and Conclusions

Calibration of parameters and validation were evaluated by way of R^2 co-efficients of determination and the Nash-Sutcliffe efficiency criterion *E* (Nash and Sutcliffe (1970). The Nash-Sutcliffe coefficient compares measured values (in this application TSS EMC's) with those predicted by a model; the coefficient *E* is calculated as:

Equation 4-7

$$E = 1 - \frac{\sum_{i=1}^{n}(M_i^{obs} - M_i^{model})^2}{\sum_{i=1}^{n}(M_i^{obs} - \bar{M}_I)^2} [-\infty|1]$$

Where:

For each observation M_i,

E = Nash-Sutcliffe co-efficient

M^{obs} = Observed TSS EMC value for n data records (mg/l)

M^{model}= Simulated TSS EMC for n data records (mg/l)

$\bar{M}_I$= Mean TSS EMC of observed data records (mg/l).

The Nash-Sutcliffe coefficient gives an indication of the model predictive accuracy, with an efficiency of 0 indicating that the model predictions are as accurate as the mean of the observed data, *E* values in the negative range show that the model has less predictive power than the mean of the observed values. The closer the model efficient value *E* is to 1, the more accuracy and thus predictive power the model has at reproducing the observed values (Nash and Sutcliffe, 1970). Calibrated parameter values and calculated Nash-Sutcliffe coefficients for each catchment are presented in Table 4-10.

Table 4-10 Parameters values and Nash Sutcliffe coefficients obtained from model calibration.

Parameters and Nash Coefficients	NW	GR	SHEP	RICH	RD	ER
b_1	32.98	15.1	36.91	97.12	69.24	52.16
b_2	160.8	65.17	76	205.1	-61.21	155.5
b_3	3158	2001.6	1103	266.9	565	222.7
b_4	99.71	32.44	56.03	74.55	18.75	43.54
λ	2.4	4.8	3.2	1.76	36.1	0.92
R^2	0.68	0.55	0.44	0.68	0.44	0.42
E	-5.05	-5.54	0.79	0.57	0.4	0.73

All six catchments were calibrated; R^2 values in the range of 0.44-0.68. Validation was considered successful in all but two catchments, Nash-Sutcliffe coefficients for successfully validated catchments in the range 0.4-0.79, this would represent a slight drop in predictive capacity when compared to the original study where all Nash-Sutcliffe coefficients were reported to be above 0.7. However, as reported by Dotto et al. (2010), when tested, many previously derived regression-based models have negative Nash-Sutcliffe values, thus the model was judged to be transferable to these catchments, this concurs with Dotto et al. (2010) hypothesis that efficient TSS pollutant models should account for explanatory factors such as antecedent climatic variables and rainfall characteristics.

The study shows that a previously published semi-empirical TSS EMC model can be used to predict TSS EMC's in catchments other than where it was first derived, strengthening the common hypothesis found in the literature that simplified water quality techniques should include some explanatory variables which account for build-up and wash off processes.

Chapter 5. Development of a new stochastic TSS EMC model

The principle objective of this thesis is to develop a new simple water quality model to be used to improve the ICM approach. Previous chapters have shown that any such model:

- Should give quantification of uncertainty associated with its predictions (Chapter 2).
- Can be used to predict event mean concentrations (Chapter 3).
- Use explanatory rainfall variables to give some account of key processes (build-up and wash-off) (Chapter 4).
- Should be transferable between catchments other than where It was developed (Chapter 4).

This aim of this chapter is to develop a new stochastic model capable of predicting storm water TSS EMC's, the chapter seeks to:

1. Identify the explanatory variables which 'best' describe variations in TSS EMC's.
2. Describe the development of a new simple TSS EMC model, the format of which incorporates build-up and wash-off processes by utilizing the explanatory variables identified in (1).
3. Investigate the use of different mathematical functions which 'best' describe the build-up and wash-off functions within the model.
4. Present a method of model calibration and validation to establish optimal parameter values and provide information on the model's predictive capabilities.
5. Present and develop an uncertainty technique which can be used within the model to quantity the uncertainty associated with its predictions.

5.1 Selection of model variables

As discussed in chapter 4, rainfall characteristics can be used as explanatory variables to describe variations in storm water quality. As part of the storm water quality monitoring campaign described in chapter 4, corresponding rainfall tipping bucket event data were analysed to enable the characterisation of rainfall variables for each of the 237 events monitored. The following rainfall event variables were derived from the data; antecedent dry weather period (ADWP); event duration (DURA); rainfall depth (DEPT); average rainfall intensity (AGI5); initial average ten-minute rainfall intensity (IT10) and corresponding TSS EMC's concentrations for each event.

With no clear academic consensus on which rainfall characteristics are 'best' for explaining variations in catchment TSS EMC's, and many possible model input variables (six), to find the rainfall variables which 'best' described variations in TSS EMC, multi-variate data analysis was required. Various multivariate analysis techniques such as principle component analysis (PCA), Cluster analysis and Discriminant analysis are described in (Miller and Miller, 2005). Due to the implementation of PCA for multivariate analysis in water quality studies within the literature, it was selected for multivariate analysis in this work (Herngren, Goonetilleke and Ayoko, 2005; Egodawatta, Thomas and Goonetilleke, 2009; Abdul Zali, Retnam and Juahir, 2011; Mohd Nasir *et al.*, 2011).

Principle component analysis (PCA) is a multivariate analysis technique often used for investigating the relationships between a multivariate data set. In this application PCA analysis was utilised to investigate the relationship between rainfall event characteristics and corresponding event TSS EMC's. The technique developed in 1901 by Karl Pearson can be used to show relationships between variables within a given data set via informative display of statistical pattern recognition. More than one variable in a data set may be measuring the same driving principle that governs the behaviours of the observational variable under investigation, thus groups of variables may 'move' together; showing correlations with one another but describing the variance of the observation variable under investigation with varying ability. By creating new principle components (PC's), linearly uncorrelated variables and groups of variables are replaced by a single new variable, thus the analytical problem is simplified. The newly created PC's are created orthogonal to one another, thus there is no redundant information, these new PC's form an orthogonal basis for the space of the data.

The first principal component is a single axis in space. When projecting each observation on this axis, the resulting values form a new variable, the variance of this variable is the maximum among all possible choices of the first axis. The second principal component is another axis in space, perpendicular to the first. Projecting the observations on this axis generates another new variable. The variance of this variable is the maximum among all possible choices of this second axis, the full set of principal components is as large as the original set of variables. It is commonplace for the sum of the variances of the first few principal components to describe most of the variance, these PC's can be subsequently analysed to determine which predictor variables or combinations of best describe the variance in the observational variable, further information on the technique can be found in (Li and Barrett, 2008).

A data matrix (237 x 6) containing all rainfall characteristic variables and corresponding TSS EMC's described in chapter 4 was created for PCA. As variables were in different units and were of varying magnitude, data were subjected to mean centring (subtraction of the mean value from each element) and standardization (individual values being divided by the standard deviation of the total variable data set) prior to PCA analysis, this pre-treatment is a common weighting technique employed to ensure all variables have equal weight in the analysis (Settle et al., 2007).

Six new PC's were created from the original variables, the most significant of these can be identfied by way of a scree plot, in which the variation of eigenvalues associated with each PC are plotted in descending order, thus showing what proportion of the variance in TSS EMC's each new PC describes (Miller and Miller, 2005) (Figure 5-1).

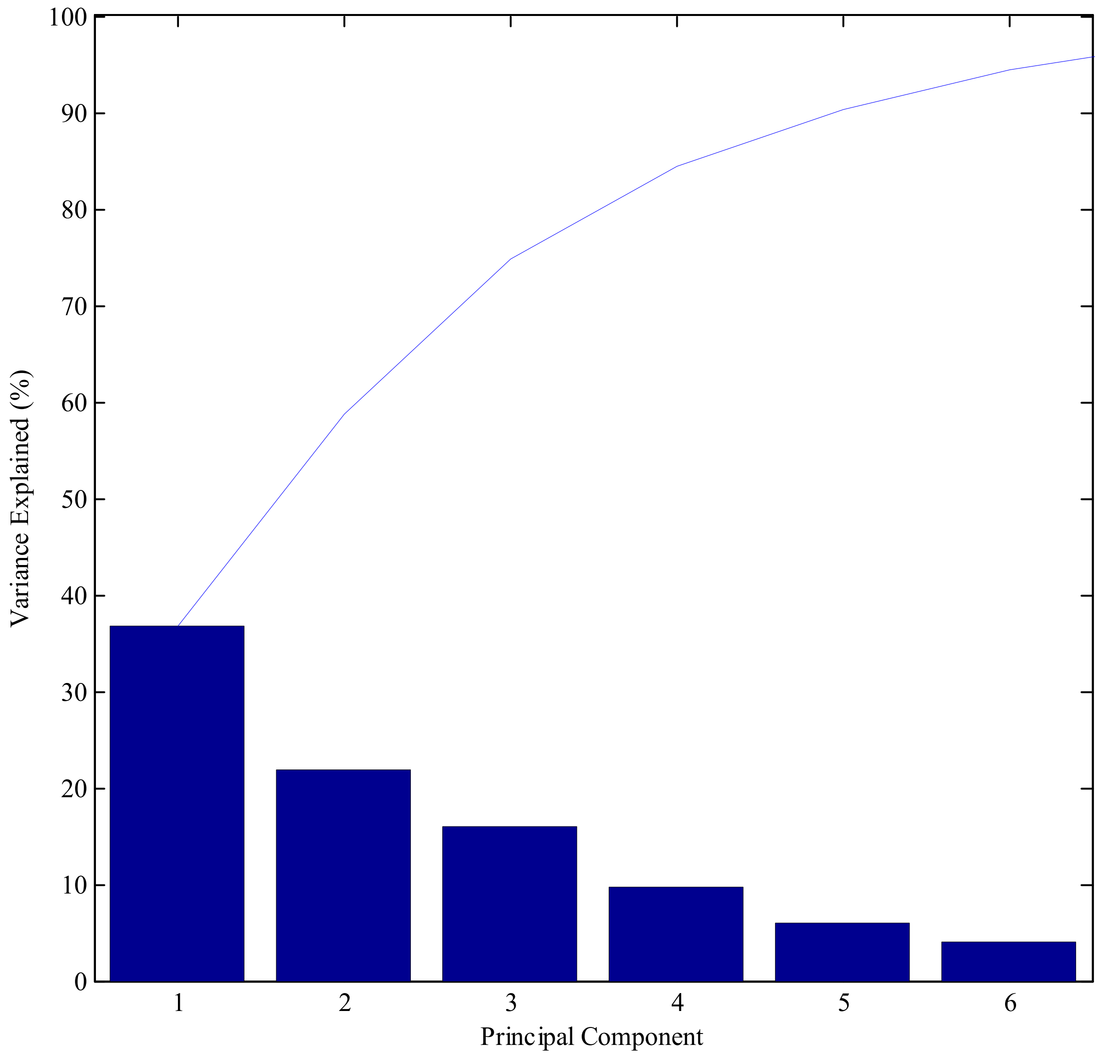

Figure 5-1 Scree plot showing what proportion of TSSEMC's variance is described by each PC.

PC1 accounts for nearly 40% of the total variance in TSS EMC's, PC1 and PC2 explain approximaltely 60% of the total variance combined, these two PC's were selected for further examination via the presentaiton of their variables through PCA bi-blots. Figure 5-2 shows the resulting PCA biplot for PC1 and PC2.

The bi-plot of the PC's show the orthonormal principle component coefficients for each variable and the respective principle component scores for each PC. In the bi-plots, vectors of each respective variable are represented by the blue lines, the length of each vector and the angles between them are indications of the correlation strength between variables; small angles indicating strong correlations, obtuse or greater angles indicate weak correlations between variables (Miller and Miller, 2005).

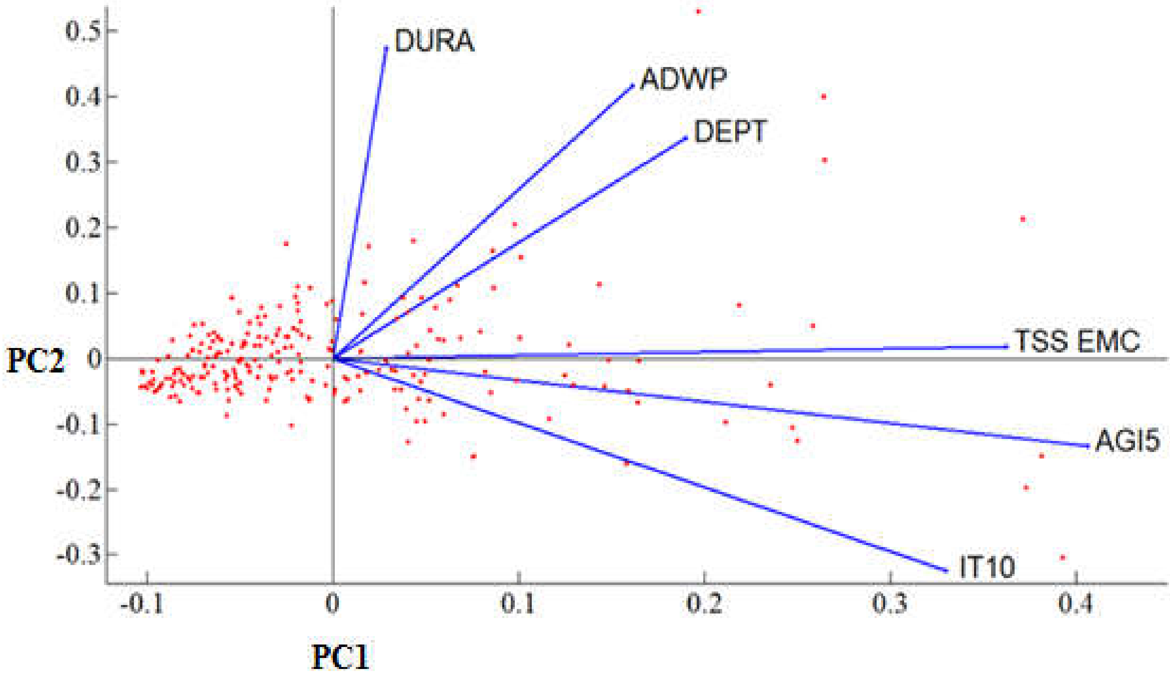

Figure 5-2 PCA bi-plot showing relationships between variables

In Figure 5-2, the angle between vectors TSS EMC and AGI5 is small, suggesting that 'average rainfall intensity' is correlated with the most standardized variation in TSS EMC concentrations, it is noted that the variables rainfall duration (DURA), antecedent dry weather period (ADWP) and rainfall depth (DEPT) show correlation with one another, as do average rainfall intensity (AGI5) and initial rainfall intensity (IT10), this would be expected as these variables are derived from the same rainfall events. ADWP is a relatively independent parameter in comparison to the five other rainfall variables, ADWP does show some correlation with TSS EMC's, the angle between these two vectors approximated to be 45 degrees.

The two key storm water processes influencing variations in TSS EMC's are build-up and wash-off. Multi-variate data analysis was performed to identify which variables could be used in a simple model to describe these processes. Due to antecedent dry weather period ADWP being the only measured variable associated with the build-up phenomena, this variable was selected for use in the model development. Of the multiple variables analysed to predict wash-off, rainfall intensity (AGI5) described the most variation in TSS EMC's and was there for selected for further use in the model development.

5.2 Model Development

Following the principal component analysis, it was hypothesised that the variation in TSS EMC's could be best described by the antecedent dry weather period preceding the event under analyses and average rainfall intensity, the two variables give some conceptual representation of build-up and wash-off processes respectively, such that TSS EMC's could be predicted be functions of these two variables.

The aim of the model is to predict average pollutant concentrations over a specified period to enable the prediction of TSS EMC's. Pollutant-wash off is most commonly replicated in storm water modelling approaches as an exponential decay equation (Egodawatta and Goonetilleke, 2008). The exponential decay equation assumes that storm water pollutant concentrations decrease exponentially with volume.

Various derivations of this equation have been utilized in well-known storm-water models such as SWMM (Tsihrintzis and Hamid, 1998). The equation has also been used to successfully develop a probabilistic storm water quality model for assessment of the 'first-flush' and in the development of stochastic approach to predicting storm water run-off during urban discharges (Bach *et al.,* 2010b and Daly *et al.,* 2014). Due to the previous successful application of this equation, it was selected for use in this work.

Considering the exponential wash-off equation in the temporal domain at the resolution of a single rainfall event, it has also been said that the pollutant concentration C decreases exponentially with respect to time (Daly *et al.*, 2014).

Equation 5-1

$$\frac{dC}{dt} = -kC$$

Where:

C = Pollutant concentration (mg/l)

k = the decay constant (s^{-1}).

This first order differential equation (Equation 5-1) can be analytically solved to provide further understanding of its behaviour. Equation 5-1 and Equation 5-2 suggest that the rate of change in pollutant concentration with respect to time is dependent on the amount of concentration currently available to be washed from the catchment surface. Equation 5-1 can be rearranged in terms of the decay constant *k* by dividing both sides by *C* as follows:

Equation 5-2

$$\frac{1}{C}\frac{dC}{dt} = -k$$

Where:

C = Pollutant concentration (mg/l)

k = the decay constant (s^{-1}).

Multiplying both sides of Equation 5-2 by *dt* yields:

Equation 5-3

$$\frac{1}{C}\, dc = \, -k\, dt$$

Where:

C = Pollutant concentration (mg/l)

k = the decay constant (s^{-1}).

Taking the integral of Equation 5-3:

Equation 5-4

$$\int_0^{\infty} \frac{1}{C}\, dC = \int_0^{\infty} -k\, dt$$

Where:

C = Pollutant concentration (mg/l)

k = the decay constant (s^{-1}).

It can be said that:

Equation 5-5

$$lnC + c_1 = -k\ t + \ c_2$$

Where:

C = pollutant concentration (mg/l)

k = the decay constant (s^{-1})

c_1 and c_2 = arbitrary constants (-).

Collecting the arbitrary constants c_1 and c_2 in Equation 5-5 gives:

Equation 5-6

$$lnC = -k\ t + c_3$$

Where:

C = pollutant concentration (mg/l)

k = the decay constant (s^{-1})

c_3 = arbitrary constant (mg/l).

By raising both sides of Equation 5-6 to the base *e*, pollutant concentration *C* can be given as a function of time:

Equation 5-7

$$e^{(\ln C)} = e^{(-kt+c_3)}$$

Where:

C = pollutant concentration (mg/l)

k = the decay constant (s^{-1})

c_3 = arbitrary constant (mg/l).

Equation 5-8

$$C = e^{-kt+c_3}$$

Where:

C = pollutant concentration (mg/l)

k = the decay constant (s^{-1})

c_3 = arbitrary constant (mg/l).

Equation 5-9

$$C = e^{-kt} e^{c_3}$$

Where:

C = pollutant concentration (-)

k = the decay constant (s^{-1})

c_3 = arbitrary constant (mg/l).

Equation 5-9

$$C(t) = c_4 e^{-kt}$$

Where:

C = pollutant concentration at time t (mg/l)

k = the decay constant (s^{-1})

c_4 = arbitrary constant (mg/l).

If the concentration of a pollutant equals zero at time = 0, substituting back into Equation 5-9, it can be said that

Equation 5-10

$$C(0) = C_0 = c_4 e^{-k\,0} = c_4 e^0 = c_4$$

C = pollutant concentration (mg/l) at time (0)

k = the decay constant (s^{-1})

c_4 = arbitrary constant (mg/l).

Thus, we are left with the following expression (Equation 5-11), which is the 'closed-form' analytical solution of Equation 5-2:

Equation 5-11

$$C_{(t)} = C_0 e^{-kt}$$

Where:

$C_{(t)}$ = the concentration of pollutant at time t (mg/l)

C_0 = the initial concentration at time (0) (mg/l)

k = the decay coefficient (s^{-1}).

With the primary output of this work being the development of a simplistic model, a model capable of producing EMC's, Equation 5-11 has been expressed graphically to show how it can be used to derive the TSS EMC (C_{mean}) of a wash-off event of duration T (Figure 5-3).

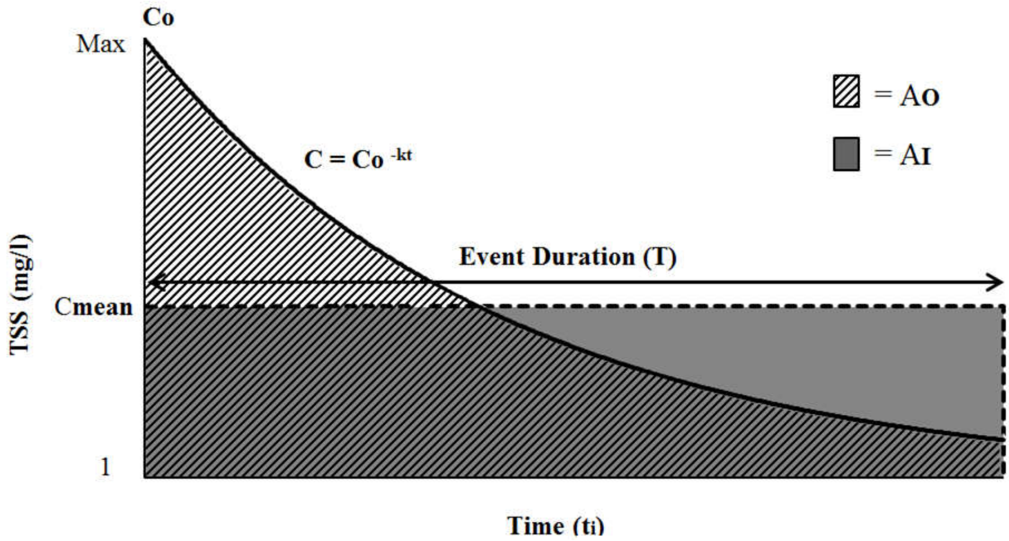

Figure 5-3 graphical event-based representation of the exponential wash-off equation

Where:

T = duration of the wash-off event (seconds)

It can be shown that for any event, the areas A_o and A_I (annotated in Figure 5-3) are considered equal, thus

Equation 5-12

$$C_{mean} = \frac{A_0}{T}$$

Where:

C_{mean} = TSS EMC (mg/l)

A_0 = Total mass over duration of event (mg s l^{-1})

T = duration of the wash-off event (s).

By integrating Equation 5-12 between limits set by the start and end times of the wash-off event under analysis (between 0 and T), it can be said that:

Equation 5-13

$$A_O = A_I = \int_0^T C_0 e^{-kT} = \frac{C_0}{-k} e^{-kT} - \frac{C_0}{-k} e^{-k0}$$

Where:

C_0 = TSS EMC at time (0) (mg/l)

A_0 = Total mass over duration of event (mg s l^{-1})

A_I = Total mass over duration of event (mg s l^{-1})

T = duration of the wash-off event (s)

k = the decay coefficient (s^{-1}).

By simplifying equation 5-14 and combining with equation 5-13, it is said that:

Equation 5-14

$$C_{mean} = \frac{1}{T} \frac{c_0}{-k} (e^{-kT} - 1)$$

Where:

C_{mean} = TSS EMC (mg/l)

C_0 = Initial TSS concentration (mg/l)

k = the decay coefficient (s^{-1})

T = duration of the wash-off event (s).

C_0 and k are hypothesized to be functions of the explanatory variables ADWP and AGI5 respectively. Following derivation of the model form, the next step in the model development process was to investigate the use of different mathematical functions for C_0 and k, utilizing the variables ADWP and AGI5 to account for the build-up and wash-off components within the model respectively.

5.2.1 Model Functions

For a given catchment, C_0 and k are assumed to be functions of the explanatory variables ADWP and AGI5 respectively, in this section, the water quality data set presented in chapter 4 is utilized to explore the different possible mathematical representations of these functions. Various regressive power and exponential functions have been used to describe pollutant build-up and wash-off loads and concentrations within the literature (Driver and Troutman, 1989; Vaze and Chiew, 2003; Dembélé *et al.*, 2011), these functions involve the use of explanatory variables and catchment specific parameter values to estimate storm water loads and concentrations. In this work, five possible functions for C_0 involving use of the explanatory variable ADWP and three possible functions for k using the explanatory variable AGI5 were selected for investigation within the model (Equation 5-14). The functions were classified with an alpha-numeric system to aid understanding during the analysis (Table 5-1), *a, b, c* and, *d* represent model parameter values.

Table 5-1 Functions selected to describe C_0 and k

Function classification number	C_0	Function classification letter	k
1	$a * ADWP^b$	A	$c * AGI5^d$
2	$a * (1 - e^{(-ADWP*b)}$	B	$c * e^{d*AGI5}$
3	$\frac{a * ADWP}{b + ADWP}$	C	$c + (AGI5 * d)$

4	$a * ln(ADWP) + b$	
5	$\frac{(a * ADWP)}{(1 + (b * ADWP)}$	

With five possible functions for C_0 (1-5) and three possible functions for *k* (A-C), a total of 15 different possible model formulations were available for trial on each catchment data set. Storm water quality event data were split randomly 80:20 for calibration and validation respectively, these events were selected at random within the mathematical programming software tool MATLAB version R2013a (www.mathworks.com).

5.2.1.1 Development of Calibration Algorithm

In order to trial the different possible model formulations, a specific calibration algorithm was developed in MATLAB, the optimization function 'fminsearch' was utilized within the algorithm. The optimization function 'fminsearch' is a commonly used optimization function utilized to find the minimum of an unconstrained multivariable function using a derivate-free method, the function was used to minimize the root-mean-square error (RMSE) between observed TSS EMC's ($C_{measured}$) and corresponding model predictions (C_{pred}) for each event.

The RMSE is a frequently used measure of the differences between values predicted by a model and those observed, the statistical parameter indicates the extent to which a model over or under-estimates measured values by aggregating the magnitudes of the errors in model prediction over all predictions into a single measure of predictive power (Miller and Miller, 2005). The RMSE is calculated as follows:

Equation 5-15

$$RMSE = \sum_{i=1}^{n} \left[\frac{Cpred_i - Cmeasured_i}{n}\right]^{\frac{1}{2}}$$

Where:

for each data point C_i,

RMSE = root-mean-square error (mg/l)

C_{pred} = TSS EMC (mg/l) predicted by the specific model formulation under analysis

$C_{measured}$ = observed TSS EMC (mg/l)

n = number of observations in the data set.

The closer the modelled results are to the observed value, the smaller the RMSE value (an RMSE value of 0 representing no error and an exact model prediction of the observed data). The algorithm iteratively changed parameter values *a,b,c* and *d* within the chosen model necessary to minimize the objective function (RMSE). For understanding, the specific calibration algorithm steps have been summarized:

1. Input calibration data variables for each catchment as vectors into Matlab
   - Observed TSS EMC's ($C_{measured}$) and corresponding variables; DURA, AGI5 and ADWP.
2. Select functions of C_0 and *k* to test within the model;
3. Set initial parameter values for model functions (*a,b,c* and *d*);
   - Various combinations of these values were iteratively trialed within the calibration algorithm until the 'fminsearch' optimization tool ran successfully. If initial parameter values were 'sufficiently' incorrect, the 'fminsearch' optimization tool within MATLAB failed.
4. Predict TSS EMC (C_{pred}) of all events in calibration data set with selected functions and initial parameters;
   - Yields vector of model predictions (C_{pred}) based on initial parameter set.
5. Calculate Root Mean Square Error (RMSE) between $C_{measured}$ and C_{pred} for all calibration events;
   - Yields RMSE value for model using initial parameter set.
6. With vector of observed values $C_{measured}$ fixed, run the optimization function 'fminsearch' to minimize the objective function RMSE by iteratively changing the initial parameter set used to yield C_{pred} in (4);
   - Yields optimal parameters in model for the catchment under analysis.
7. Re-run C_{pred} using optimal model parameter set and present final RMSE values.

- Yields final RMSE value representative of how well the optimized model predicted observed TSS EMC's.

The calibration algorithm was applied to each of the catchments presented in chapter 4, optimal parameter values for each possible model formulation and associated RMSE values are presented in Table 5-2 to Table 5-7.

Table 5-2 Calibrated Model formulation, optimal parameter sets and respective RMSE values for ER catchment (Optimal model formulation highlighted in bold).

Model	C_o	k	a	b	c	d	RMSE
1A	$a * ADWP^b$	$c * AGI5^d$	21.8	0.71	0.0007	0.5	25.7
2A	$a * (1 - e^{(-ADWP*b)})$	$c * AGI5^d$	111	-0.25	0.007	0.007	26.9
3A	$\frac{a * ADWP}{b + ADWP}$	$c * AGI5^d$	210	38.83	-0.07	-1.4	26.9
4A	$a * \ln(ADWP) + b$	$c * AGI5^d$	125.2	2.12	0.072	-1.5	21.7
5A	$\frac{a * ADWP}{1 + (b * ADWP)}$	$c * AGI5^d$	56.72	0.031	0.063	-1.4	26.9
1B	$a * ADWP^b$	$c * e^{d*AGI5}$	87	0.46	0.01	-0.001	30.3
2B	$a * (1 - e^{(-ADWP*b)})$	$c * e^{d*AGI5}$	253	-27	0.06	-0.3	27.1
3B	$\frac{a * ADWP}{b + ADWP}$	$c * e^{d*AGI5}$	436	3.9	0.04	-0.36	27.0
4B	$\boldsymbol{a * \ln(ADWP) + b}$	$\boldsymbol{c * e^{d*AGI5}}$	131	1.70	0.04	-0.34	21.1
5B	$\frac{a * ADWP}{1 + (b * ADWP)}$	$c * e^{d*AGI5}$	111	0.25	0.04	-0.3	27.1
1C	$a * ADWP^b$	$c + (AGI5 * d)$	108	0.34	0.0129	-0.0011	30.4
2C	$a * (1 - e^{(-ADWP*b)})$	$c + (AGI5 * d)$	944	-0.04	0.012	-0.001	32.3

3C	$\frac{a * ADWP}{b + ADWP}$	$c + (AGI5 * d)$	212	0.645	0.013	-0.0012	31.0
4C	$a * \ln(ADWP) + b$	$c + (AGI5 * d)$	95	2.3	0.013	-0.0011	29.3
5C	$\frac{a * ADWP}{1 + (b * ADWP)}$	$c + (AGI5 * d)$	328	1.54	0.0156	-0.012	31.0

Table 5-3 Calibrated Model formulation, optimal parameter sets and respective RMSE values for GR catchment (Optimal model formulation highlighted in bold).

Model	C_o	k	a	b	c	d	RMSE
1A	$a * ADWP^{b}$	$c * AGI5^{d}$	46	0.31	0.0005	-0.475	37.7
2A	$a * (1 - e^{(-ADWP * b)})$	$c * AGI5^{d}$	204	0.024	0.0061	-0.077	50.2
3A	$\frac{a * ADWP}{b + ADWP}$	$c * AGI5^{d}$	99	1.62	0.001	0.24	37
4A	$a * \ln(ADWP) + b$	$c * AGI5^{d}$	37	2.18	0.007	0.32	36.8
5A	$\frac{a * ADWP}{1 + (b * ADWP)}$	$c * AGI5^{d}$	61	0.614	0.001	0.24	37.9
1B	$a * ADWP^{b}$	$c * e^{d * AGI5}$	46	0.26	0.006	0.0466	38.5
2B	$a * (1 - e^{(-ADWP * b)})$	$c * e^{d * AGI5}$	68	-17.3	0.002	-0.412	39.3
3B	$\frac{a * ADWP}{b + ADWP}$	$c * e^{d * AGI5}$	32	3.61	0.005	-0.0075	38.3
4B	$\boldsymbol{a * \ln(ADWP) + b}$	$\boldsymbol{c * e^{d * AGI5}}$	37	1.95	0.0011	0.0298	35.1
5B	$\frac{a * ADWP}{1 + (b * ADWP)}$	$c * e^{d * AGI5}$	53	0.51	0.0014	0.0263	37.9
1C	$a * ADWP^{b}$	$c + (AGI5 * d)$	16	0.319	0.0014	0.0040	78.1
2C	$a * (1 - e^{(-ADWP * b)})$	$c + (AGI5 * d)$	63	-42	0.007	-0.0001	39.7

3C	$\frac{a*ADWP}{b+ADWP}$	$c+(AGI5*d)$	69	0.216	0.0002	-0.0001	39.6
4C	$a*\ln(ADWP)+b$	$c+(AGI5*d)$	32	3.79	0.0001	-0.0001	38.1
5C	$\frac{a*ADWP}{1+(b*ADWP)}$	$c+(AGI5*d)$	319	4.62	0.0002	-0.0001	39.6

Table 5-4 Calibrated Model formulation, optimal parameter sets and respective RMSE values for NW catchment (Optimal model formulation highlighted in bold).

Model	C_o	k	a	b	c	d	RMSE
1A	$a*ADWP^b$	$c*AGI5^d$	137	0.05	0.002	-0.93	69.2
2A	$a*(1-e^{(-ADWP*b)})$	$c*AGI5^d$	111	-5.2	0.0001	6.1	76.5
3A	$\frac{a*ADWP}{b+ADWP}$	$c*AGI5^d$	139	0.087	0.0029	-0.969	69.7
4A	$a*\ln(ADWP)+b$	$c*AGI5^d$	49	13.4	0.0027	-0.952	69.1
5A	$\frac{a*ADWP}{1+(b*ADWP)}$	$c*AGI5^d$	1.59	0.0115	0.0001	-0.0008	69.7
1B	$a*ADWP^b$	$c*e^{d*AGI5}$	130	-0.001	0.0053	-0.463	67.9
2B	$a*(1-e^{(-ADWP*b)})$	$c*e^{d*AGI5}$	130	-66.9	0.0054	-0.489	65.4
3B	$\frac{a*ADWP}{b+ADWP}$	$c*e^{d*AGI5}$	128	0.0013	0.0019	0.0053	69.8
4B	$a*\ln(ADWP)+b$	$c*e^{d*AGI5}$	53	11.69	0.0044	-0.406	67.9
5B	$\frac{a*ADWP}{1+(b*ADWP)}$	$c*e^{d*AGI5}$	1.06	0.0074	0.007	0.01	69.1
1C	$a*ADWP^b$	$c+(AGI5*d)$	137	0.132	0.0034	0.0008	79.2
2C	$a*(1-e^{(-ADWP*b)})$	$c+(AGI5*d)$	116	-369	0.005	-0.001	63.5

3C	$\boldsymbol{\frac{a * ADWP}{b + ADWP}}$	$\boldsymbol{c + (AGI5 * d)}$	112	-0.009	0.0051	-0.002	63.4
4C	$a * \ln(ADWP) + b$	$c + (AGI5 * d)$	15	2.692	0.000	-0.000	63.5
5C	$\frac{a * ADWP}{1 + (b * ADWP)}$	$c + (AGI5 * d)$	579	0.0495	0.000	-0.000	64.3

Table 5-5 Calibrated Model formulation, optimal parameter sets and respective RMSE values for RCW catchment (Optimal model formulation highlighted in bold).

Model	C_o	k	a	b	c	d	RMSE
1A	$a * ADWP^b$	$c * AGI5^d$	148	0.49	0.030	-1.29	52.6
2A	$a * (1 - e^{(-ADWP*b)})$	$c * AGI5^d$	493	-0.25	0.031	-0.132	55.1
3A	$\frac{a * ADWP}{b + ADWP}$	$c * AGI5^d$	673	4.7	0.033	-1.27	54.7
4A	$a * \ln(ADWP) + b$	$c * AGI5^d$	172	1.52	0.029	-1.28	52.6
5A	$\frac{a * ADWP}{1 + (b * ADWP)}$	$c * AGI5^d$	142	0.21	0.031	-1.27	54.7
1B	$a * ADWP^b$	$c * e^{d*AGI5}$	109	0.20 7	0.0029	-0.03	66.7
2B	$a * (1 - e^{(-ADWP*b)})$	$c * e^{d*AGI5}$	150	-2.95	0.0030	0.05	69.8
3B	$\frac{a * ADWP}{b + ADWP}$	$c * e^{d*AGI5}$	164	0.27	0.0031	0.003	68.5
4B	$\boldsymbol{a * \ln(ADWP) + b}$	$\boldsymbol{c * e^{d*AGI5}}$	172	1.54	0.054	-0.510	34.2
5B	$\frac{a * ADWP}{1 + (b * ADWP)}$	$c * e^{d*AGI5}$	148	0.23	0.06	-0.525	51.9
1C	$a * ADWP^b$	$c + (AGI5 * d)$	135	0.14	0.0029	0.007	67.8
2C	$a * (1 - e^{(-ADWP*b)})$	$c + (AGI5 * d)$	149	-3.02	0.0031	0.0001	69.7
3C	$\frac{a * ADWP}{b + ADWP}$	$c + (AGI5 * d)$	164	0.27	0.0030	0.000	68.5
4C	$a * \ln(ADWP) + b$	$c + (AGI5 * d)$	73	2.74	0.0031	-0.003	66.3

5C	$\frac{a * ADWP}{1+(b * ADWP)}$	$c + (AGI5 * d)$	601	3.65	0.0030	0.000	68.5

Table 5-6 Calibrated Model formulation, optimal parameter sets and respective RMSE values for RICH catchment (Optimal model formulation highlighted in bold).

Model	C_o	k	a	b	c	d	RMSE
1A	$a * ADWP^b$	$c * AGI5^d$	121	0.28	0.0028	0.0086	72.6
2A	$a * (1 - e^{(-ADWP*b)})$	$c * AGI5^d$	144	-4.7	0.0015	-0.132	79.2
3A	$\frac{a * ADWP}{b + ADWP}$	$c * AGI5^d$	176	0.22	0.0022	-0.091	77.7
4A	$a * \ln(ADWP) + b$	$c * AGI5^d$	90	2.3	0.0024	-0.006	69.8
5A	$\frac{a * ADWP}{1+(b * ADWP)}$	$c * AGI5^d$	786	4.4	0.0022	-0.09	76.4
1B	$a * ADWP^b$	$c * e^{d*AGI5}$	120	0.27	0.0030	0.0194	72.6
2B	$a * (1 - e^{(-ADWP*b)})$	$c * e^{d*AGI5}$	319	-0.19	0.0032	0.0704	83.7
3B	$\frac{a * ADWP}{b + ADWP}$	$c * e^{d*AGI5}$	165	0.17	0.0023	0.0039	77.5
4B	$\boldsymbol{a * \ln(ADWP) + b}$	$\boldsymbol{c * e^{d*AGI5}}$	78	2.01	0.014	-1.17	60.4
5B	$\frac{a * ADWP}{1+(b * ADWP)}$	$c * e^{d*AGI5}$	847	4.1	0.0052	-0.188	77.3
1C	$a * ADWP^b$	$c + (AGI5 * d)$	294	0.37	0.0119	0.0073	78.6
2C	$a * (1 - e^{(-ADWP*b)})$	$c + (AGI5 * d)$	139	-5.14	0.011	0.0003	78.5
3C	$\frac{a * ADWP}{b + ADWP}$	$c + (AGI5 * d)$	162	0.18	0.0014	0.0004	77.4
4C	$a * \ln(ADWP) + b$	$c + (AGI5 * d)$	85	2.45	0.0016	0.0005	71.5
5C	$\frac{a * ADWP}{1+(b * ADWP)}$	$c + (AGI5 * d)$	881	5.44	0.0014	0.0004	77.4

Table 5-7 Calibrated Model formulation, optimal parameter sets and respective RMSE values for SHEP catchment (Optimal model formulation highlighted in bold).

Model	C_0	k	a	b	c	d	RMSE
1A	$a * ADWP^b$	$c * AGI5^d$	95	0.28	0.0058	-2.87	60.6
2A	$a * (1 - e^{(-ADWP*b)})$	$c * AGI5^d$	224	-4.7	0.0015	-0.132	57.5
3A	$\frac{a * ADWP}{b + ADWP}$	$c * AGI5^d$	192	0.67	0.0069	-2.52	58
4A	$a * \ln(ADWP) + b$	$c * AGI5^d$	47	2.16	-0.001	1.397	62.3
5A	$\frac{a * ADWP}{1 + (b * ADWP)}$	$c * AGI5^d$	287	1.49	0.0069	-0.52	58.1
1B	$a * ADWP^b$	$c * e^{d*AGI5}$	48	0.38	-0.0003	0.2981	65.0
2B	$a * (1 - e^{(-ADWP*b)})$	$c * e^{d*AGI5}$	195	-1.29	0.0044	0.0025	68.4
3B	$\frac{a * ADWP}{b + ADWP}$	$c * e^{d*AGI5}$	197	0.60	0.0033	0.0025	68.6
4B	$a * \ln(ADWP) + b$	$c * e^{d*AGI5}$	45	2.03	0.0004	0.2542	64.3
5B	$\frac{a * ADWP}{1 + (b * ADWP)}$	$c * e^{d*AGI5}$	393	1.7	0.0749	-1.232	55.9
1C	$a * ADWP^b$	$c + (AGI5 * d)$	2.43	2.25	2.022	-0.0886	68.6
2C	$\boldsymbol{a * (1 - e^{(-ADWP*b)})}$	$\boldsymbol{c + (AGI5 * d)}$	180	-0.96	0.0057	-0.0013	55.4
3C	$\frac{a * ADWP}{b + ADWP}$	$c + (AGI5 * d)$	196	0.95	0.0050	-0.0011	56.0
4C	$a * \ln(ADWP) + b$	$c + (AGI5 * d)$	70	1.58	0.0031	-0.0008	58.4
5C	$\frac{a * ADWP}{1 + (b * ADWP)}$	$c + (AGI5 * d)$	205	1.04	0.0050	-0.0011	56.0

For simplicity, the most effective model formulations and RMSE characteristics derived for each catchment have been presented in Table 5-8.

Table 5-8 Summary of RMSE values generated during model calibration

	Min RMSE	Model form	RMSE Range	Mean RMSE
ER	21.1	4B	21.1 – 32.3	27.64
GR	35.1	4B	35.1 – 78.1	41.58
NW	63.4	3C	63.4 -79.2	68.5
RCW	34.2	4B	34.2 - 69.8	60.1
RICH	60.4	4B	60.4 -79.2	75.4
SHEP	55.4	2C	55.4 – 68.6	60.9

Following derivation of optimal parameters from calibration, model formulation 4B was found to be the most effective form of model across catchments ER, GR, RCW and RICH, yielding RMSE values of 21.1, 35.1, 34.2 and 60.4 respectively. Model formulations 3C and 2C yielded the RMSE values of 63.4 and 55.4 for catchments NW and SHEP respectively. Based on the results presented in Table 5-2 - Table 5-7, model formulation 4B was judged to be the most effective at describing variations in TSS EMC's across all catchments, thus the final model formulation (4B) is presented, with C_0 and k defined as:

Equation 5-16

$$C_0 = a * \ln(ADWP) + b$$

Where:

C_0 = Initial TSS (mg L^{-1}) concentration at time (0)

$ADWP$ = antecedent dry weather period (s)

a and b = calibration parameters (mg L^{-1}).

Equation 5-17

$$k = c * e^{d*AGI5}$$

Where:

k = decay coefficient (s^{-1})

$AGI5$ = average rainfall intensity (mm/s)

c = calibration parameter (s^{-1})

d = calibration parameter (-).

The model can be presented in its final form:

Equation 5-18

$$C_{mean} = \frac{1}{T}\frac{a * \ln(ADWP) + b}{c * e^{d*AGI5}}(e^{-c*e^{d*AGI5}*T} - 1)$$

Where:

C_{mean} = TSS EMC (mg/l)

T = duration of the wash-off event (s)

$AGI5$ = average rainfall intensity (mm/hr)

$ADWP$ = antecedent dry weather period (hr)

a = calibration parameter (mg/l)

b = calibration parameter (mg/l)

c = calibration parameter (s^{-1})

d = calibration parameter (-)

Optimized parameter values for the final model for each catchment are presented in Table 5-9.

Table 5-9 Optimised catchment parameter values generated for calibration of model formulation 4B.

	a	b	c	d	RMSE
ER	131	1.70	0.04	-0.34	21.1
GR	37	1.95	0.0011	0.0298	35.1
NW	53	11.69	0.0044	-0.4055	67.9
RCW	172	1.54	0.054	-0.5101	34.2
RICH	78	2.01	0.014	-1.17	60.4
SHEP	45	2.03	0.0004	0.2542	64.3

Calibration plots using the final model form and optimised parameter values for each respective catchment are presented in Figure 5-4, Figure 5-5, Figure 5-6, Figure 5-7, Figure 5-8 and Figure 5-9.

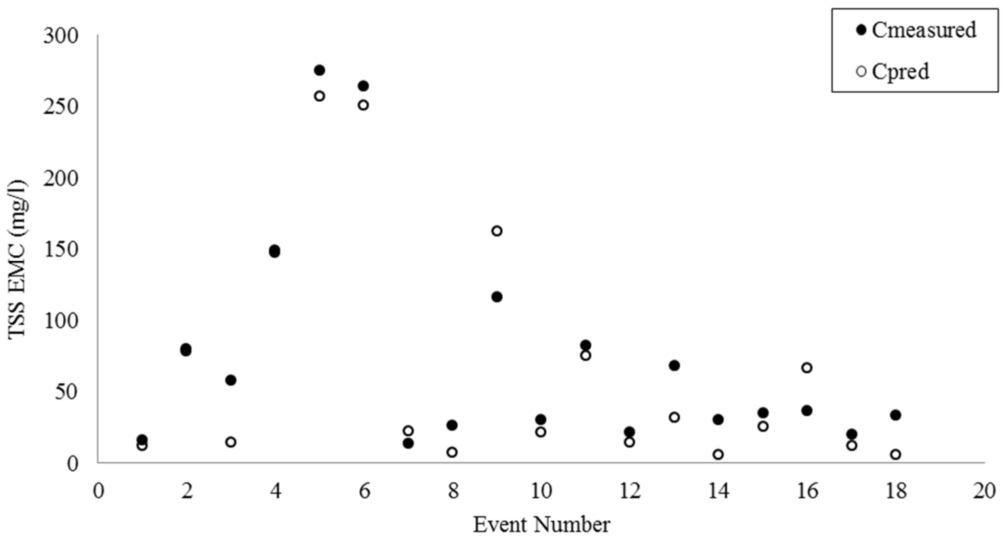

Figure 5-4 Calibration plot for ER catchment showing difference in model calibration predictions (Cpred) and measured EMC's (Cmeasured)

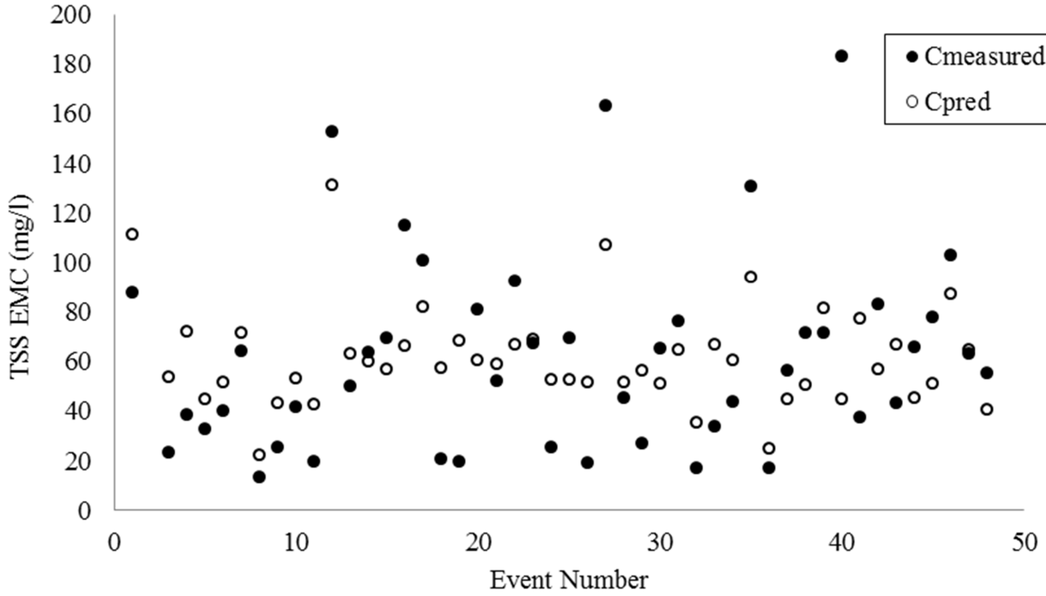

Figure 5-5 Calibration plot for GR catchment showing optimised model calibration predictions (Cpred) and measured EMC's (Cmeasured)

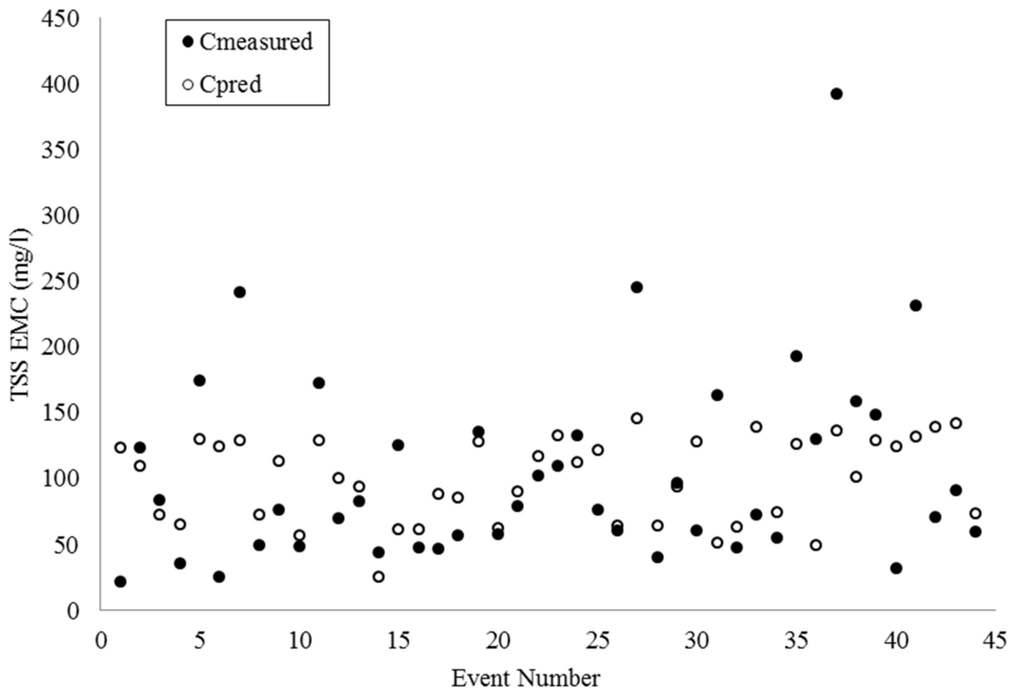

Figure 5-6 Calibration plot for NW catchment showing optimised model calibration prediction (Cpred) and measured EMC's (Cmeasured)

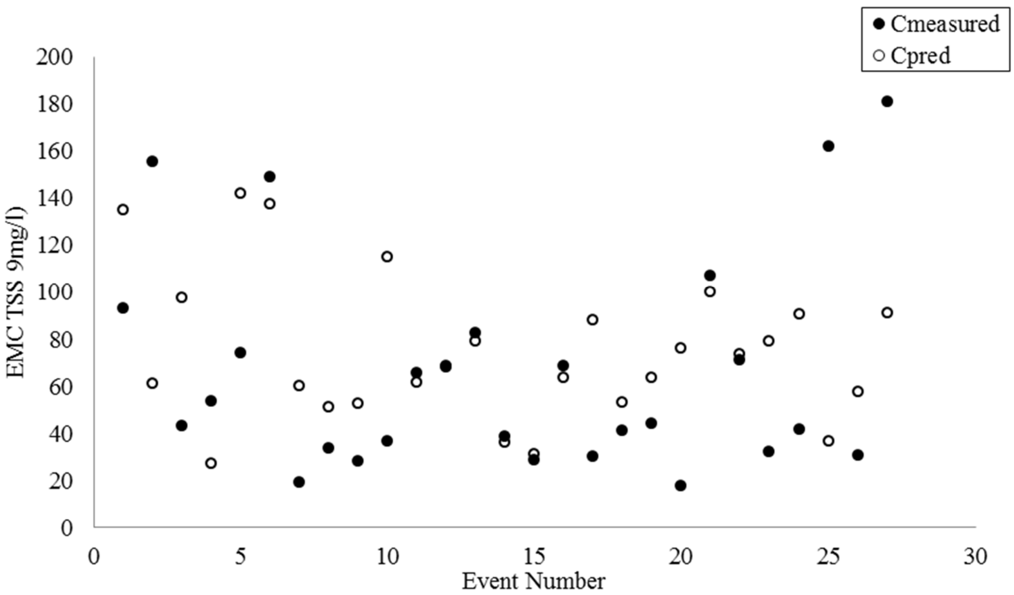

Figure 5-7 Calibration plot for RCW catchment showing optimised model calibration predictions (Cpred) and measured EMC's (Cmeasured)

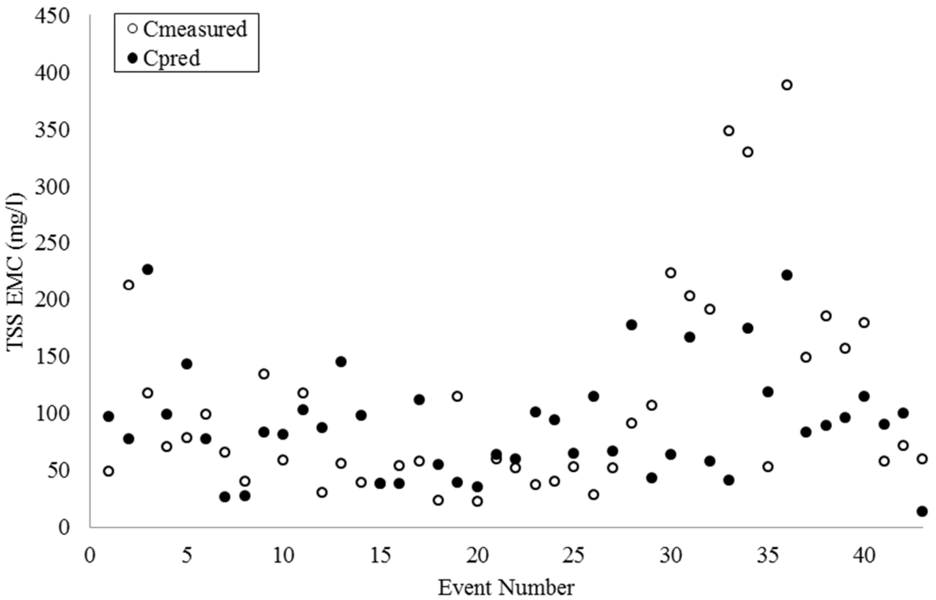

Figure 5-8 Calibration plot for RICH catchment showing optimised model calibration predictions (Cpred) and measured EMC's (Cmeasured)

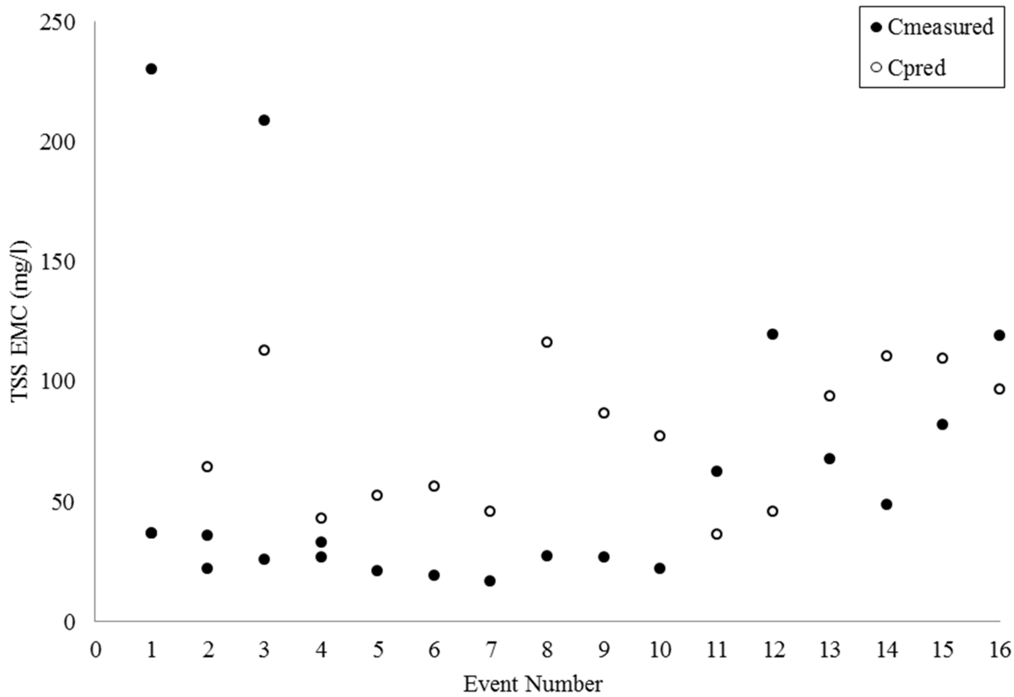

Figure 5-9 Calibration plot for SHEP catchment showing optimised model calibration predictions (Cpred) and measured EMC's (Cmeasured)

Following calibration of each catchment model, validation of the model was carried out on the remaining 20% of each respective data set; these results are discussed together at the end of this chapter, validation plots for each respective catchment (ER, GR, RCW, NW, RICH and SHEP) are presented in Figure 5-10, Figure 5-11, Figure 5-12, Figure 5-13, Figure 5-14 and, Figure 5-15.

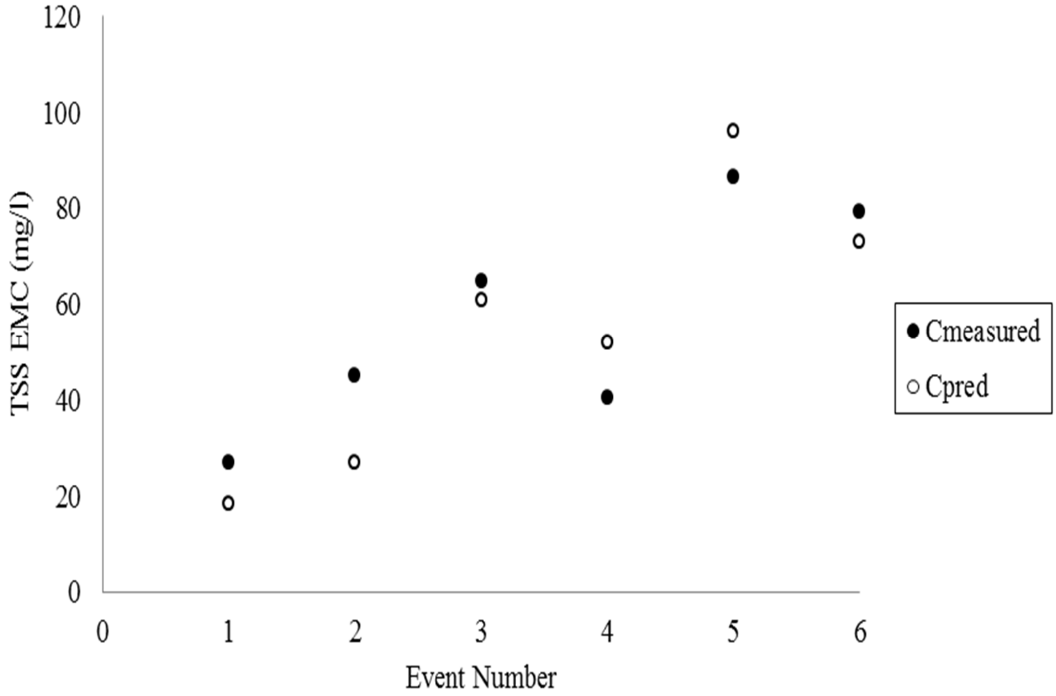

Figure 5-10 Validation plot for ER catchment showing calibrated model predictionsTSS EMC’s (Cpred) and measured TSS EMC’s (Cmeasured)

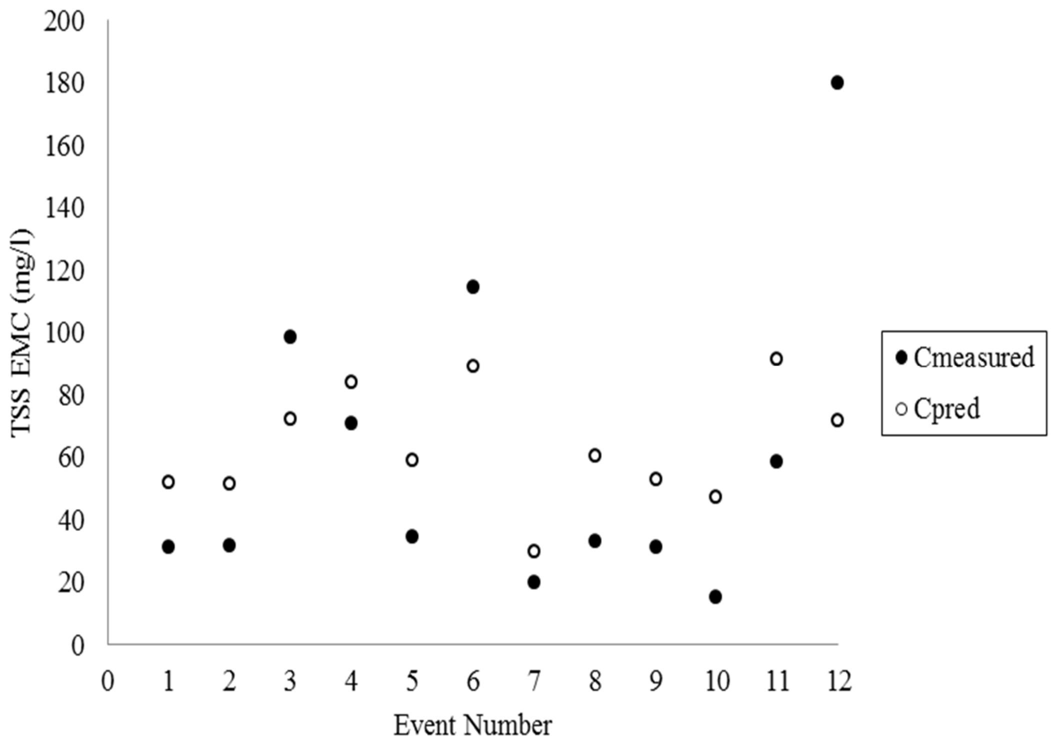

Figure 5-11 Validation plot for GR catchment showing calibrated model predictions (Cpred) and measured EMC’s (Cmeasured)

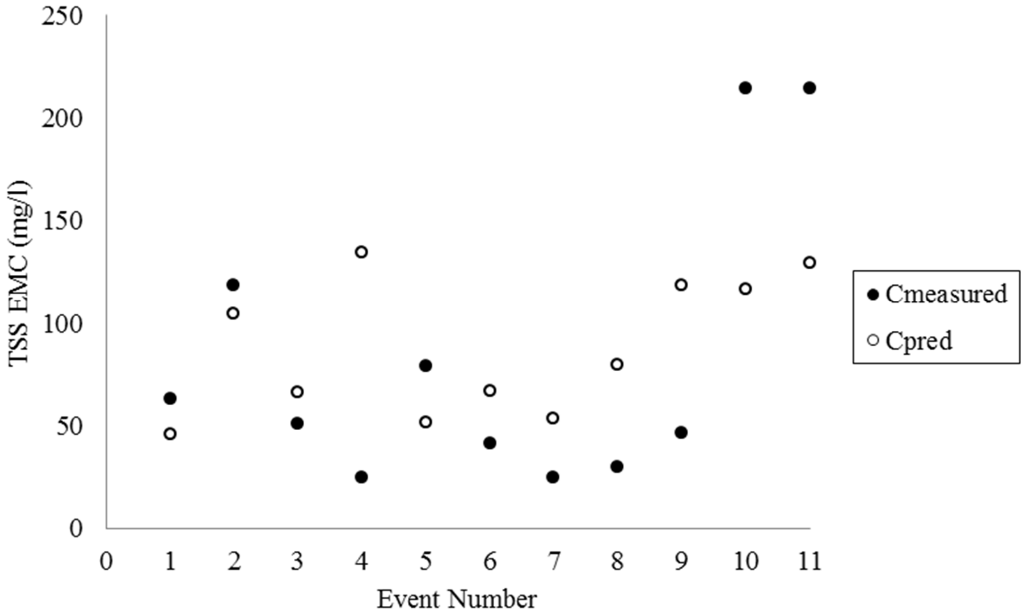

Figure 5-12 Validation plot for NW catchment showing calibrated model predictions (Cpred) and measured EMC's (Cmeasured)

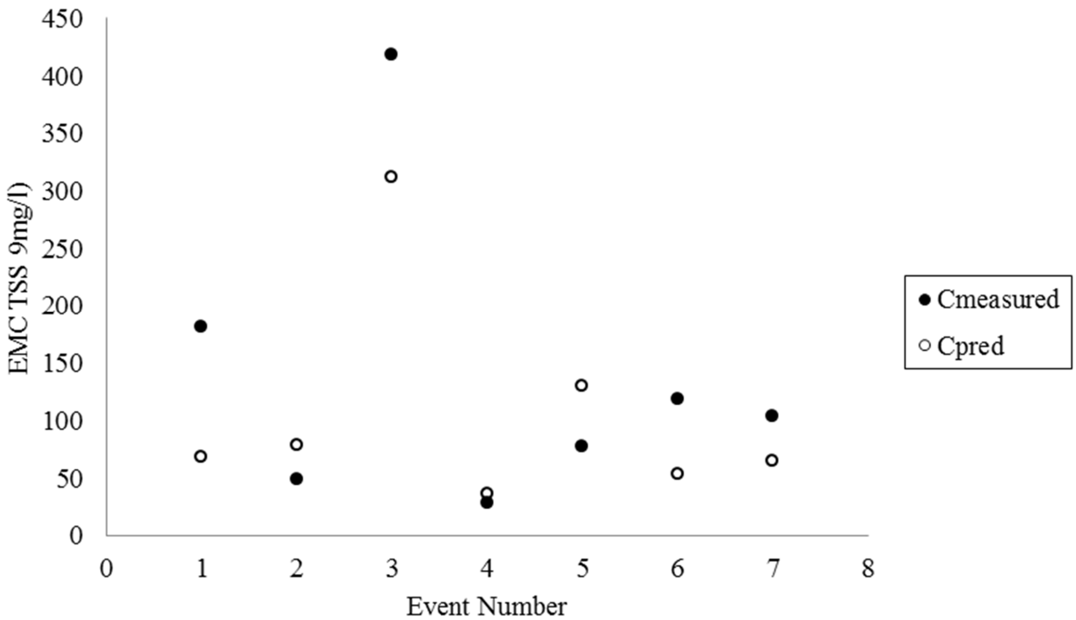

Figure 5-13 Validation plot for RCW catchment showing calibrated model predictions (Cpred) and measured EMC's (Cmeasured)

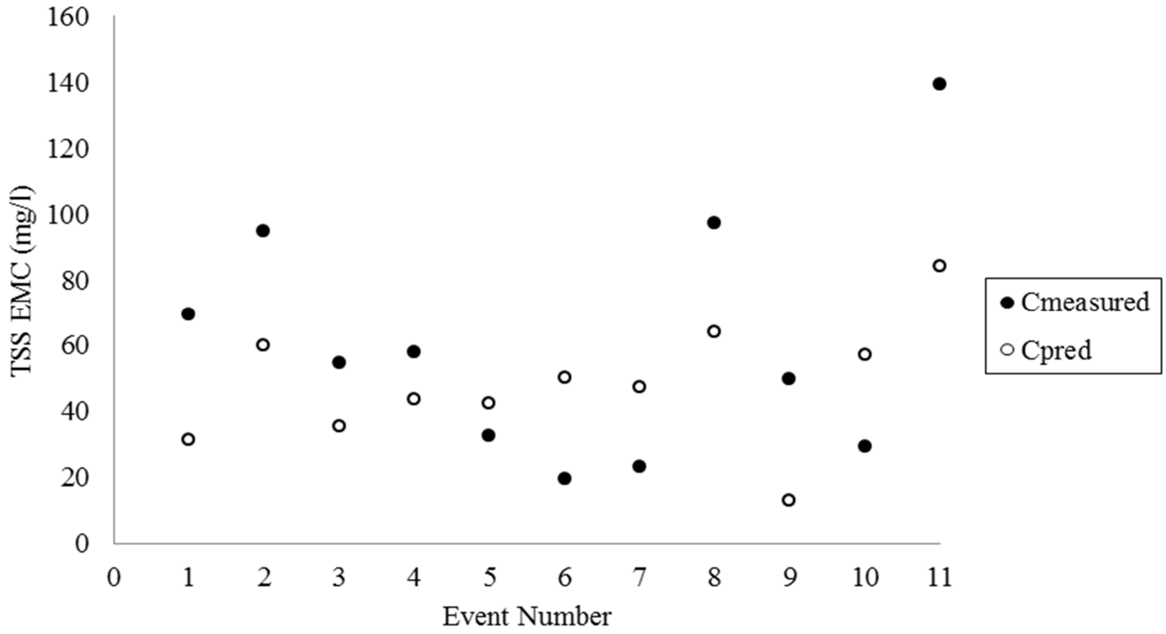

Figure 5-14 Validation plot for RICH catchment showing calibrated model predictions (Cpred) and measured EMC's (Cmeasured)

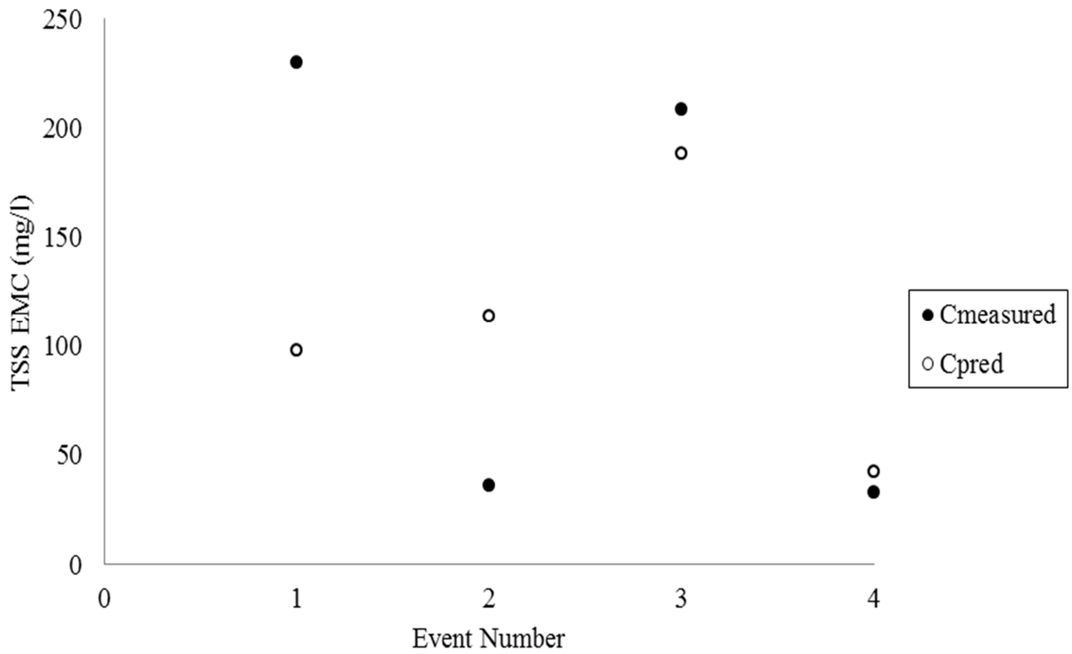

Figure 5-15 Validation plot for SHEP catchment showing calibrated model predictions (Cpred) and measured EMC's (Cmeasured)

The Nash-Sutcliffe coefficient was used to evaluate the calibration and validation model efficiencies E presented in Table 5-10. It is noted that the RMSE was previously used within the calibration algorithm presented to optimise parameter values, whilst both the RMSE and Nash-Sutcliffe coefficient can be used to evaluate model efficiencies, it was concluded that the Nash-Sutcliffe efficiency value was required to adjudge the predictive performance of the model to allow comparison with other models cited within the literature (Dotto *et al*., 2011), this is presented in the discussion and conclusions section of this chapter.

Table 5-10 Nash-Sutcliffe model efficiencies for calibration and validation

	Calibration		Validation	
	No of events	Calibration (E)	No of events	Validation (E)
ER	18	0.81	6	0.85
GR	48	0.63	12	0.32
NW	44	0.18	11	0.26
RCW	27	0.68	7	0.66
RICH	43	0.38	11	0.19
SHEP	16	0.41	4	0.67

Model validation E values were in the range 0.18 – 0.81, mean calibration and validation E values were 0.51 and 0.49 respectively.

5.3 Model Sensitivity

In this section, a review of sensitivity analysis techniques is presented, subsequently, a global sensitivity analysis methodology has been applied to allow for a sensitivity evaluation of the TSS EMC model developed in section 5.2, discussion of the results is presented in the discussion and conclusions section of this chapter 5.5.

An evaluation of model output confidence is good practise following the development of any scientific model (Dotto *et al.*, 2012). Sensitivity analyses allow for such evaluation by showing the relevance of model inputs in determining variations in model outputs. The potential benefits of such an evaluation to model developers are as follows (Dotto *et al.*, 2011; Vanrolleghem *et al.*, 2015):

- Increased understanding of the relationships between outputs and input variables.
- Identification of model inputs that need attention should the modeller seek to increase model robustness.
- To enable the simplification of model structure and the potential to fix or remove parts of the model which are redundant.
- To improve calibration through the understanding of model parameters; often data collection for model calibration is limited, thus understanding of influential parameters (those which model outputs are sensitive too) is useful.

Sensitivity analyses can be broadly categorized as either global or local. Local sensitivity analysis can be used to understand the effect of model input perturbations on model outputs; these types of analyses differ from global sensitivity analysis (GSA) techniques in that they are performed around a single point in the model parameter space. Global sensitivity analyses can be performed over the whole parameter space of model inputs, allowing for a greater understanding of how model input parameter sets impact model outputs. There exists a variety of possible methods to globally analyse model parameter sensitivity, the selection of which is linked to the objectives of the analysis, in this work, the objectives of the analysis are:

- To detect the influence of model parameter on model outputs; allowing fixing or the utilisation of default values for parameters which are not influential on model outputs, subsequently, model simplification can be performed;
- To understand the potential impact of model input uncertainty, allowing future calibration campaigns to be focussed on influential model inputs.
- To understand the interactions between model inputs and parameters.

Commonly used examples of GSA techniques cited within the literature are:

- Standard Regression Co-efficient method (SRC) (Saltelli, 2002).
- Extended-FAST method (Saltelli, 2002).

- Morris Screening method (Morris, 1991).
- Sobol' indices (Sobol, 2001).

Several model attributes should be considered when selecting an appropriate GSA methodology, typically; the number of input and model parameters being assessed, the computation cost of running the model and the length of each model simulation (Vanrolleghem *et al.*, 2015). With respect to the TSS EMC model the number of model variable and parameters is small (seven), the computational cost low and the model run time speed low; the model performs one simulation in less than a second in the numerical software package Matlab version R2013a (www.mathworks.com). The application of GSA techniques within the urban drainage modelling field is limited due to high computational costs of such procedures (Dotto *et al.*, 2010). Vanrolleghem *et al.,* (2015) suggested that when used to examine the sensitivity of a conceptual water quality simulation model, SRC, Extended-FAST and Morris screening methods produced similar results, subsequently, the Morris screening method has been selected for GSA in this work.

Morris Screening

In this work, the input and model parameters selected for sensitivity analysis are: Rainfall event duration (T); rainfall event Intensity (mm/hr); antecedent dry weather period (ADWP) and model parameters *a*,*b*,*c* and *d* for the build-up and wash-off components of the model. As the model is newly developed, model parameter ranges selected for the sensitivity analysis were taken to be the minimum and maximum values of each respective input and parameter sets recorded from the field data and during the process of model development respectively. Table 5-11 presents the ranges of input and model parameters considered for sensitivity analysis. Model input and parameter values were sampled from a uniform distribution within their respective ranges to achieve even and uniform representation within the parameter space.

Table 5-11 Input and Model Parameters and Ranges used in the Global Sensitivity Analysis

Input and model Parameters	Unit	Minimum	Maximum
Rainfall event duration	mins	12	1409
Antecedent dry weather period	Days	0.08	46
Rainfall Intensity	mm/hr	0.1	30.1
a	-	45	172
b	-	1.54	11.69
c	-	0.004	0.064
d	-	-1.17	-0.25

The Morris' method samples large factoral spaces by following several trajectories, such trajectories are selected one-at-at-time (OAT) in a discretized manner within parameter levels. Initial trajectories start at a random point in the factoral space (defined by a combination of modalities of all factors points). In a step-wise manner, the trajectory of exploration is then determined by the OAT procedure involving successful variations of factor modalities, thus each trajectory can be defined as p+1 possible combination of factor modalities.

For this study, the parameter space was partitioned into *p* discrete levels and random sampling performed to generate *r* Elementary Effects (EE). The number of simulations required for the screening procedure can be calculated by $r * (n + 1)$, where *n* is the number of model parameters considered for the analysis. Campolongo *et al.*, (2005) proposed a modification to the Morris screening procedure via the use of an absolute mean (μ^*) utilized as an improved measure of sensitivity. A similar approach to the use of the Morris screening approach and Campolongo *et al.,* (2005) modification is presented in Sriwastava *et al.*, (2018) to quantify the uncertainty in sewerage model variable and input parameters. In this application, for parameter sensitivity quantification, the absolute mean $\mu^*$and standard deviation σ of EE's need be defined. A high value of μ^* suggests that the model outputs are highly sensitive to a change in each parameter. A high value of σ indicates non- linearity and/or parameter interaction which affected model output variability. For this study, the parameter space was discretized into *p*=20 levels and the number of repetitions, r= 100, thus 800 simulations were required for the analysis.

Morris Screening Results

In this study, as presented in Vanrollegham, at al. (2015) and Sriwastava *et al.*, (2018), convergence analysis has been performed by examining the percentage change in variability of a sensitivity index value S_{sc}, the sensitivity index value S_{sc} is given by:

Equation 5-19

$$S_{sc} = \frac{\sum_{i=1}^{NF} SC_i}{NF}$$

Where:

S_{sc} = sensitivity index value

NF = the number of input parameters

SC_i = the sensitivity index of parameter i.

The variability of the index (y) is given by:

Equation 5-20

$$y = \left[\frac{\sum_{i=1}^{NF} SC_{i_{n_k-1}} - \sum_{i=1}^{NF} SC_{i_{n_k}}}{NF}\right]$$

Where:

S_{sc} = sensitivity index value

NF = the number of input parameters

SC_i = the sensitivity index of parameter i

n_k = the number of simulations.

To determine the number of simulations required for different output variables Vanrollegham, at al. (2015) applied a precision threshold of the range 0.5% to

3.5%. In this study, a precision threshold of 0.1% was achieved after 300 or more simulation. Morris screening procedure results are presented in Table 5-12, inputs and parameters have been ranked according to their μ^* values. Discussion and conclusions associated with the results of the GSE are presented in section 5.9.

Table 5-12 Morris screening results and ranking of input/model parameters.

Parameters	Absolute mean (μ^*)	Rank
c	0.1729	1
Rainfall intensity	0.1711	2
Rainfall event duration	0.1431	3
a	0.0157	4
Antecedent dry weather period	0.0080	5
d	0.0059	6
b	0.0027	7

5.4 Model Uncertainty

Chapter 2 introduced the concept of uncertainty and some of the various methods which have been used to quantify uncertainty of urban drainage modelling predictions. This section uses the water quality data set presented in chapter 4 and the final model formulations to quantify uncertainties associated with the predictions made by the newly developed TTS EMC, this was achieved by study of the errors associated with the model's predictions ($C_{predicted}$) and observed values (C_{measured}). The method assumes that the models input, calibration and structural uncertainties are described by the error between model predictions of TSS EMC's ($C_{predicted}$) and observed TSS EMC's (C_{measured}), the study of these errors can be used to develop a simple uncertainty technique for use with the newly developed model presented in section 5.2. The method is referred to in this work as the ‘factor-ratio’ uncertainty method utilising probability distributions associated with model prediction errors and a Monte Carlo simulation estimate the uncertainty associated with model predictions; a similar approach was utilised by Schellart (2008) to quantify the impact of uncertainty in sediment transport equations. Discussions regarding the implication of the assumptions made in the development and application of this method are presented in chapter 7.

‘Factor Ratio’ Uncertainty Methodology

The method predicts model output uncertainty by utilising probability distributions for the ratio of error (C_{ratio}) of the newly developed model predictions ($C_{predicted}$) and (C_{measured}).

In probability theory, a probability distribution (pdf) is a mathematical function which provides the probabilities of occurrences of different possible outcomes associated with an experiment (Li and Hyman, 2004), a cumulative distribution function (cdf) of a random variable (*x*), evaluated at *x,* represents the probability that the random variable will take a value less than or equal to *x* (Pianosi and Wagener, 2015).

All data fitting was performed using the software package Matlab version R2013a (www.mathworks.com). The software contains a built-in statistic toolbox for exploratory data and distribution analyses. The distribution fitting tool within this tool box (dfitool) was used within this work, the tool allows users to fit several distributions to their data; evaluate the ‘goodness of fit’ of such distributions through visual interpretation and descriptive statics (necessary for objective interpretation) and subsequently create distribution objects. The distribution tool uses maximum likelihood estimation to fit distributions to data (Matlab Documentation, 2013).

The tool allows users to examine the following possible fits:

- Beta (unit interval values) distribution, fit using the function betafit.
- Binomial (nonnegative values) distribution, fit using the function binopdf.
- Birnbaum-Saunders (positive values) distribution.
- Burr Type XII (positive values) distribution.

- Exponential (nonnegative values) distribution, fit using the function expfit.
- Extreme value (all values) distribution, fit using the function evfit.
- Gamma (positive values) distribution, fit using the function gamfit.
- Generalized extreme value (all values) distribution, fit using the function gevfit.
- Generalized Pareto (all values) distribution, fit using the function gpfit.
- Inverse Gaussian (positive values) distribution.
- Logistic (all values) distribution.
- Loglogistic (positive values) distribution.
- Lognormal (positive values) distribution, fit using the function lognfit.
- Nakagami (positive values) distribution.
- Negative binomial (nonnegative values) distribution, fit using the function nbinpdf.
- Nonparametric (all values) distribution, fit using the function ksdensity.
- Normal (all values) distribution, fit using the function normfit.
- Poisson (nonnegative integer values) distribution, fit using the function poisspdf.
- Rayleigh (positive values) distribution using the function raylfit.
- Rician (positive values) distribution.
- t location-scale (all values) distribution.
- Weibull (positive values) distribution using the function wblfit.

Subsequently, the package allows users to perform Monte-Carlo sampling procedures from distribution objects necessary to derive confidence intervals (a range of values so defined that there is a specified probability that the value of a parameter lies within it) around each model prediction (Kreutz, Raue and Timmer, 2012). The steps carried out to attain these intervals for the Factor Ratio method is presented:

1. Calculate model residuals using Equation 5-21

Equation 5-21

$$Residual\ Error_i = Cpredicted_i - Cmeasured_i$$

Where:

for the event *i,*

$Residual\ Error$ = model residual error (mg/l)

$C_{predicted}$ = the model prediction of TSS EMC (mg/l)

$C_{measured}$ = the measured TSS EMC (mg/l).

2. Standardize model residuals to generate new variable C_{ratio} using Equation 5-22

Equation 5-22

$$\frac{Cpredicted_i}{Cmeasured_i} = Cratio_i$$

Where:

for the event *i,*

$Cratio$ = ratio of error (-)

$C_{predicted}$ = the model prediction of TSS EMC (mg/l)

$C_{measured}$ = the measured TSS EMC (mg/l).

3. Fit probability distribution function to variable C_{ratio}.
4. Sample from C_{ratio} using Monte-Carlo procedure to gain new vector of error (V_{error}).
5. Multiply model prediction by V_{error} to generate new vector of possible EMC's ($P_{Possible}$).
6. Fit probability distribution $P_{Possible}$ to generate new pdf ($U_{\mathrm{Predicted}}$) associated with specific model prediction.
7. Compute specified confidence intervals from U_{Pred} to generate uncertainty bounds associated with model prediction.

Due to data scarcity, calibration and validation data sets were combined for the Factor-Ratio uncertainty method; the implications of this are discussed in chapter 7.

Residual errors were calculated using Equation 5-21. The method has been applied to the data for individual catchments (ER, GR, NW, RCW, RICH and SHEP) and to a collation of all six catchments data, the new data set is referred to as ‘combined’. Plots of each catchments residual error (Including error for the combined data) are presented in Figure 5-16, Figure 5-17, Figure 5-18, Figure 5-19, Figure 5-20, Figure 5-21 and, Figure 5-22.

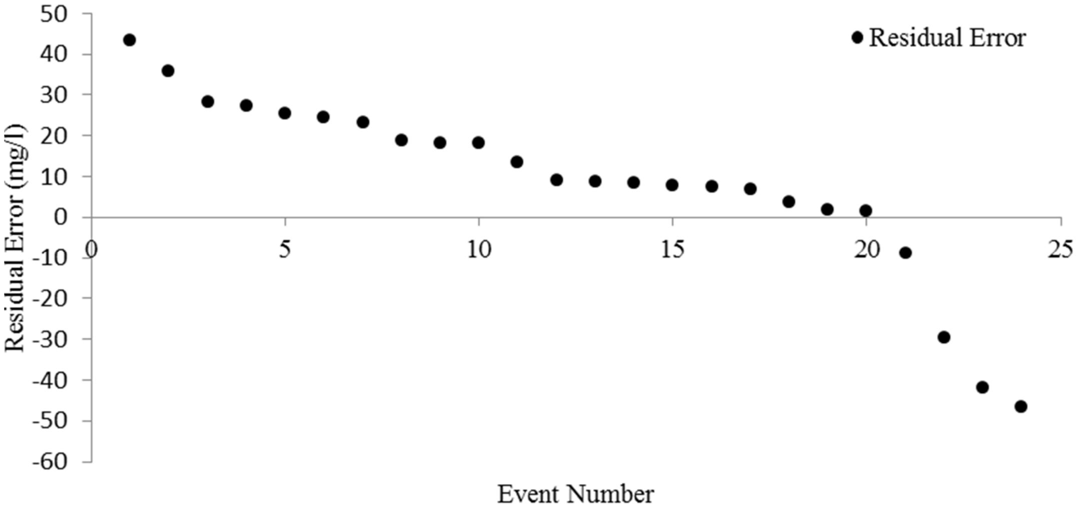

Figure 5-16 Residual error plot for ER catchment showing error between predicted TSS EMC’s (Cpredicted) and measured TSS EMC’s (Cmeasured).

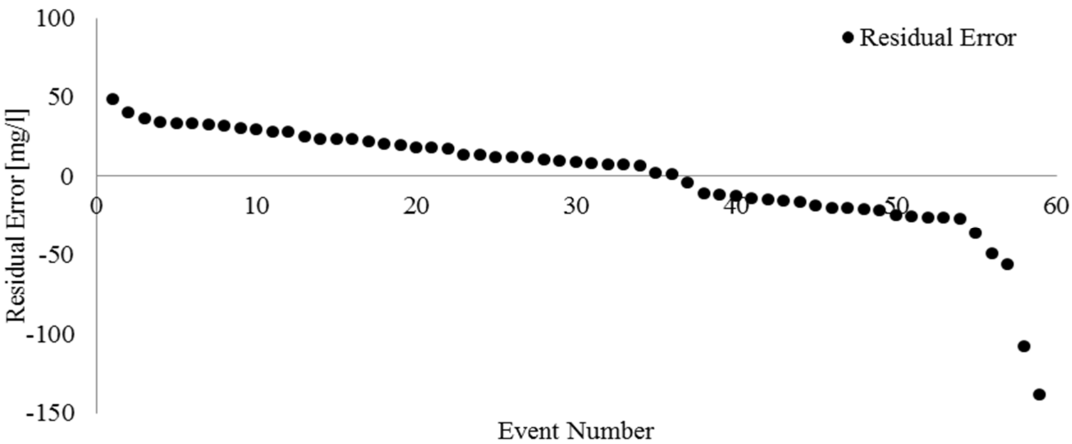

Figure 5-17 Residual error plot for GR catchment showing error between predicted TSS EMC’s (Cpredicted) and measured TSS EMC’s (Cmeasured).

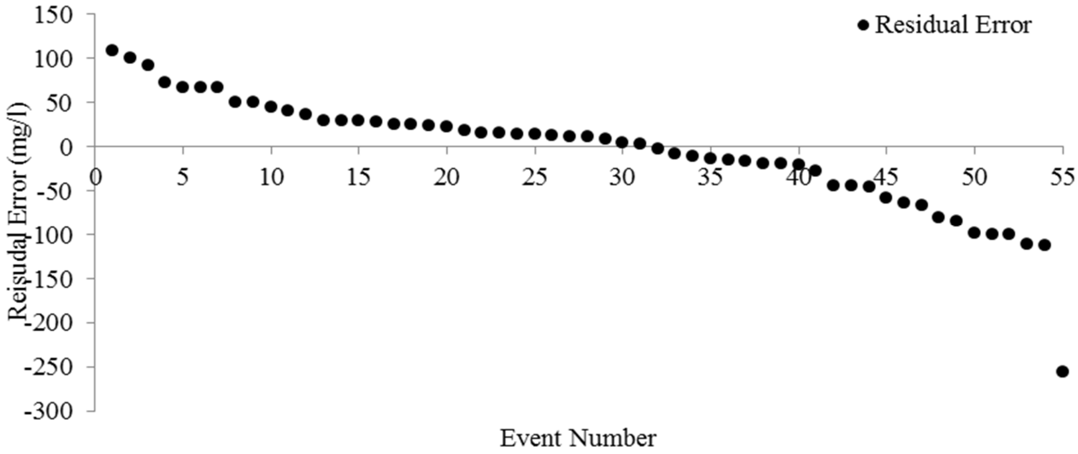

Figure 5-18 Residual error plot for NW catchment showing error between predicted TSS EMC's (Cpredicted) and measured TSS EMC's (Cmeasured).

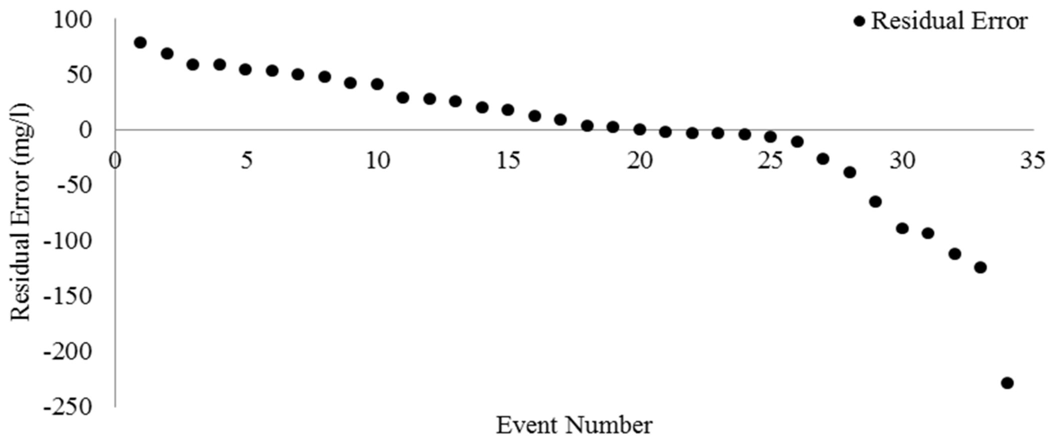

Figure 5-19 Residual error plot for RCW catchment showing error between predicted TSS EMC's (Cpredicted) and measured TSS EMC's (Cmeasured).

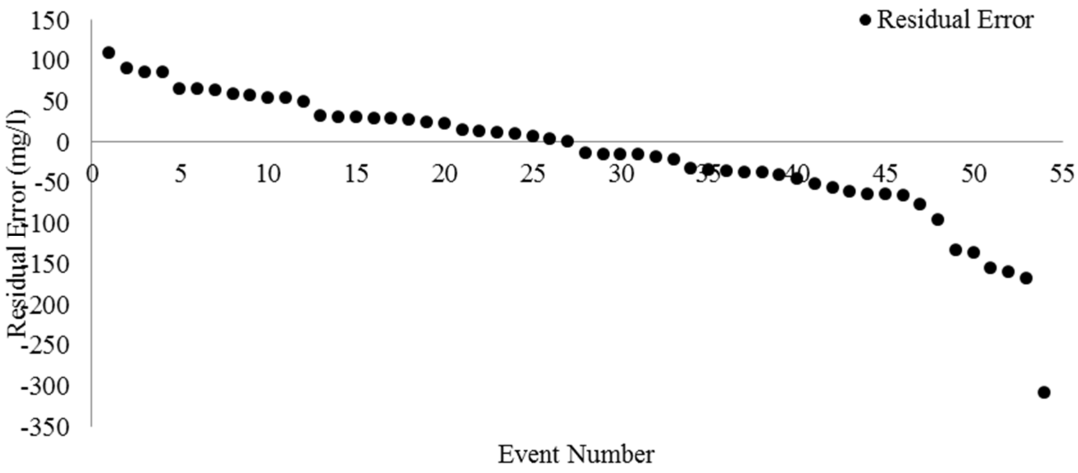

Figure 5-20 Residual error plot for RICH catchment showing error between predicted TSS EMC's (Cpredicted) and measured TSS EMC's (Cmeasured).

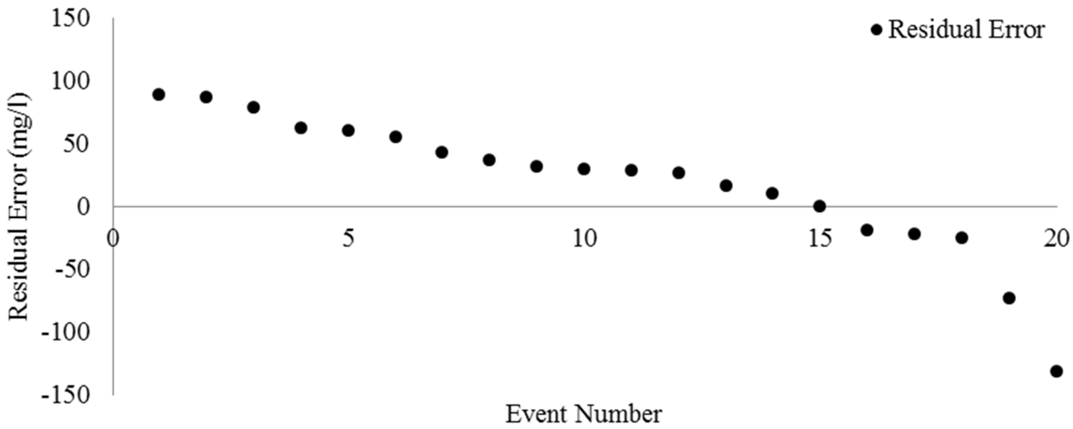

Figure 5-21 Residual error plot for SHEP catchment showing error between predicted TSS EMC's (Cpredicted) and measured TSS EMC's (Cmeasured).

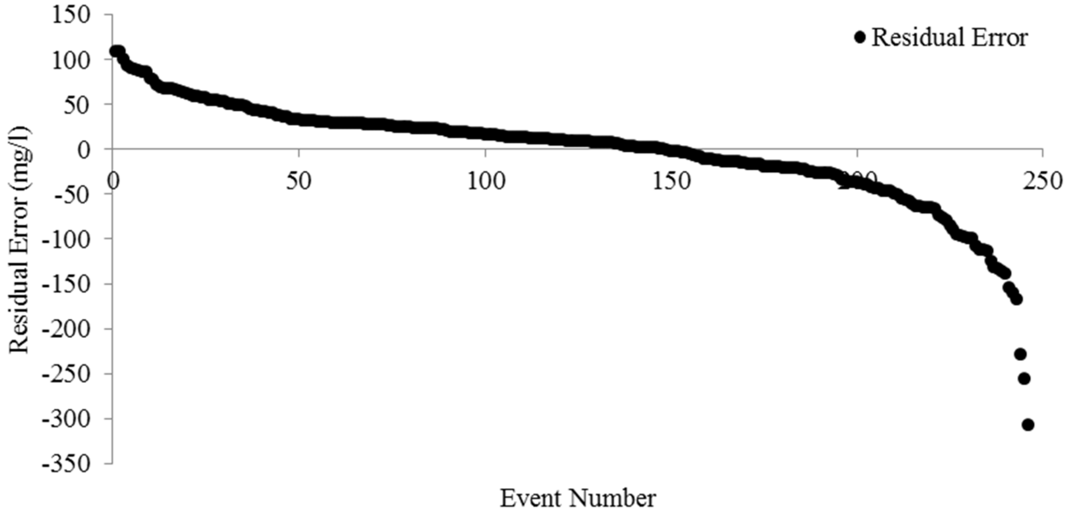

Figure 5-22 Residual error plot for combined catchment data showing error between predicted TSS EMC's (Cpredicted) and measured TSS EMC's (Cmeasured).

Cumulative probability density functions for all catchment and the combined catchment data set are presented in Figure 5-23 and Figure 5-24 respectively.

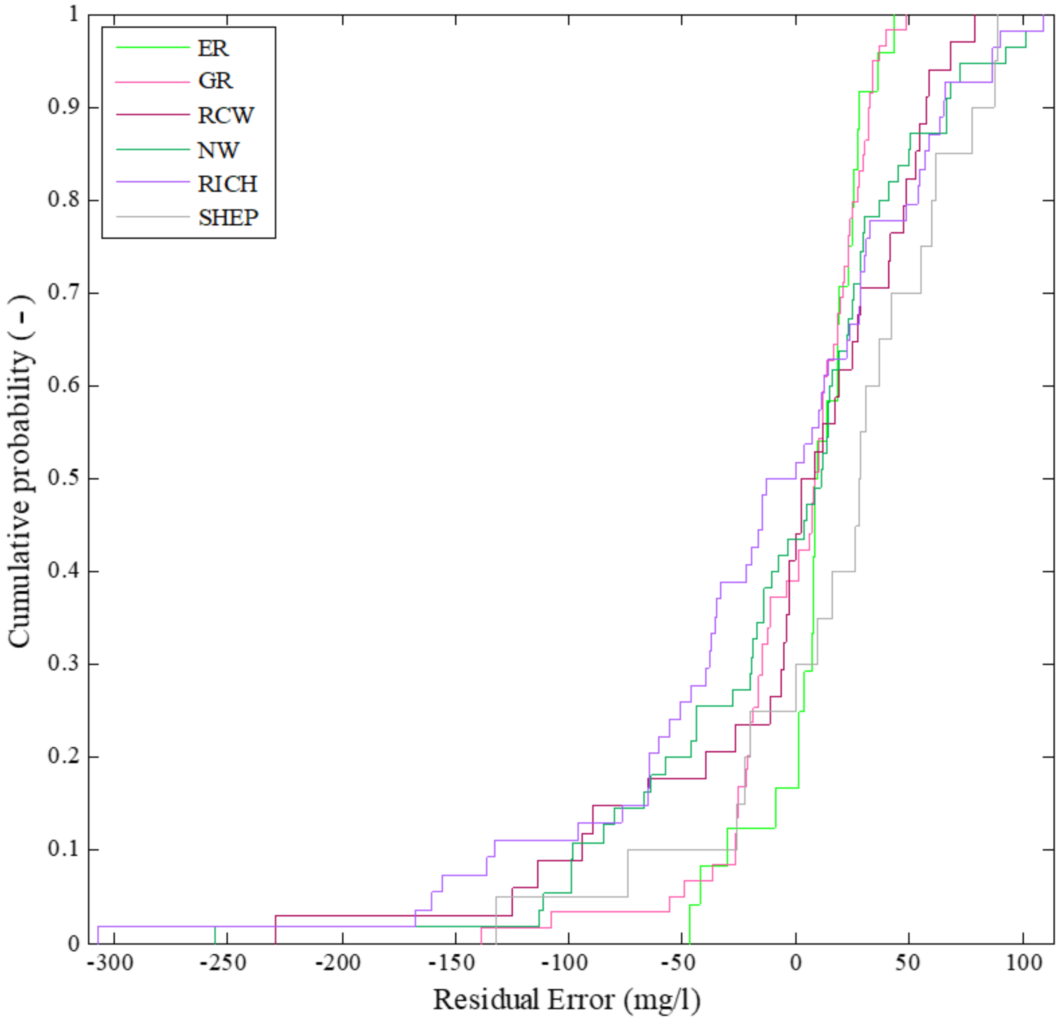

Figure 5-23 Cumulative density functions of residual error for ER, GR, RCW, NW, RICH and SHEP catchments.

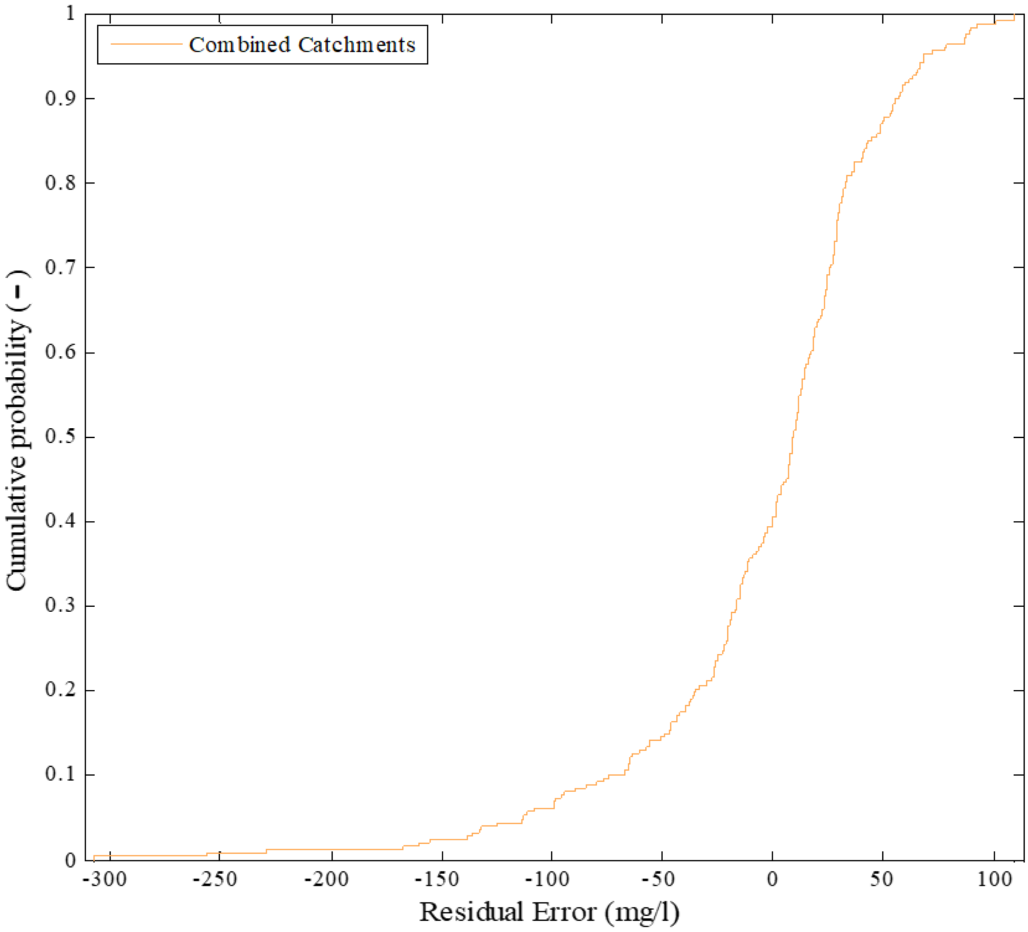

Figure 5-24 Cumulative density functions of residual error for combined catchment data set.

Table 5-13 shows the average model residual error (expressed at 50% cumulative probability) for each catchment and the combined data set.

Table 5-13 Average error extracted from CDF's

	ER	GR	NW	RCW	RICH	SHEP	Combined
Average error	8.9	8.5	10.3	-4.2	-4	28	9

To standardize model residuals in accordance with the Factor Ratio uncertainty procedure described, a new variable (C_{ratio}) was created using Equation 5-22. Normality plots of catchment $C_{ratio(s)}$ were created to determine whether the model residuals showed departures from normality. In a normal probability plot, deviations from the straight line imposed on the plot (representative of normally distributed data) show a departure from normality (Ryan and Joiner, 1976). Figure 5-25, Figure 5-26, Figure 5-27, Figure 5-28, Figure 5-29 and, Figure 5-30 show normality plots of $C_{ratio(s)}$ for each respective catchment, Figure 5-31 shows the normality plot of combined C_{ratio} values across all combined catchments.

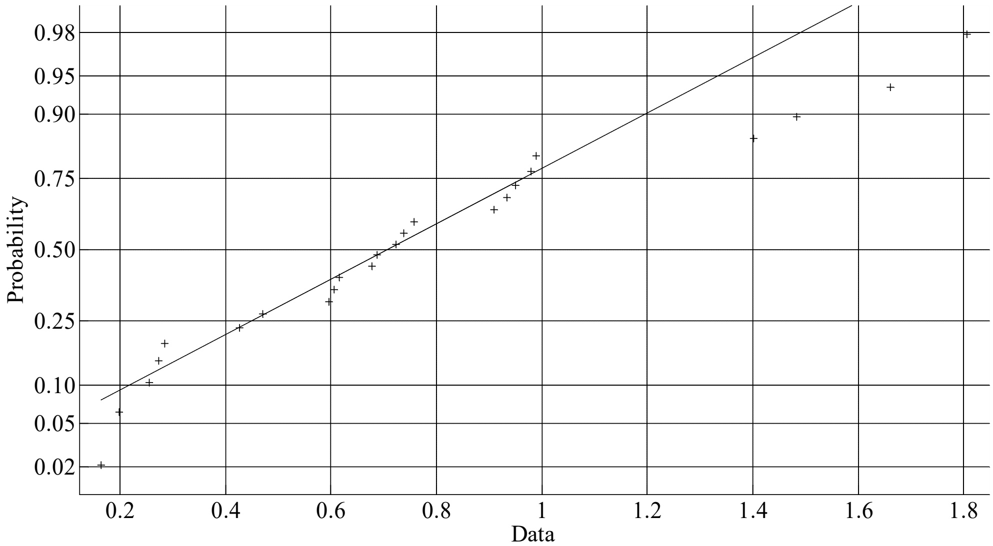

Figure 5-25 Normality plot for the ER catchment, $C_{ratio(s)}$ values shown as 'Data' on the x axis.

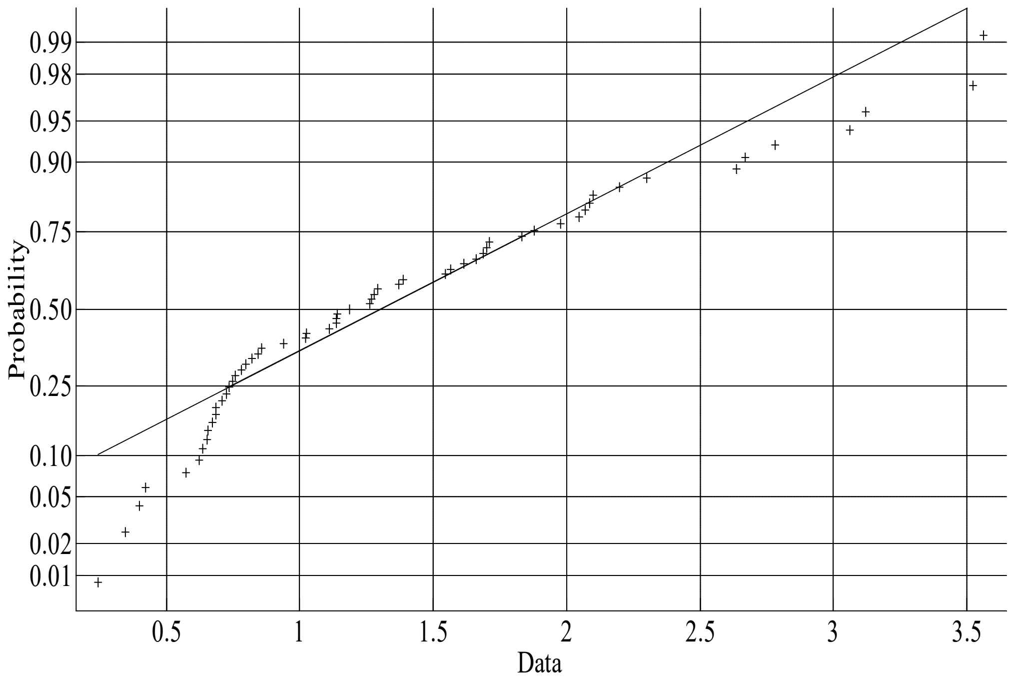

Figure 5-26 Normality plot for the GR catchment, $C_{ratio(s)}$ shown as 'Data' on the x axis.

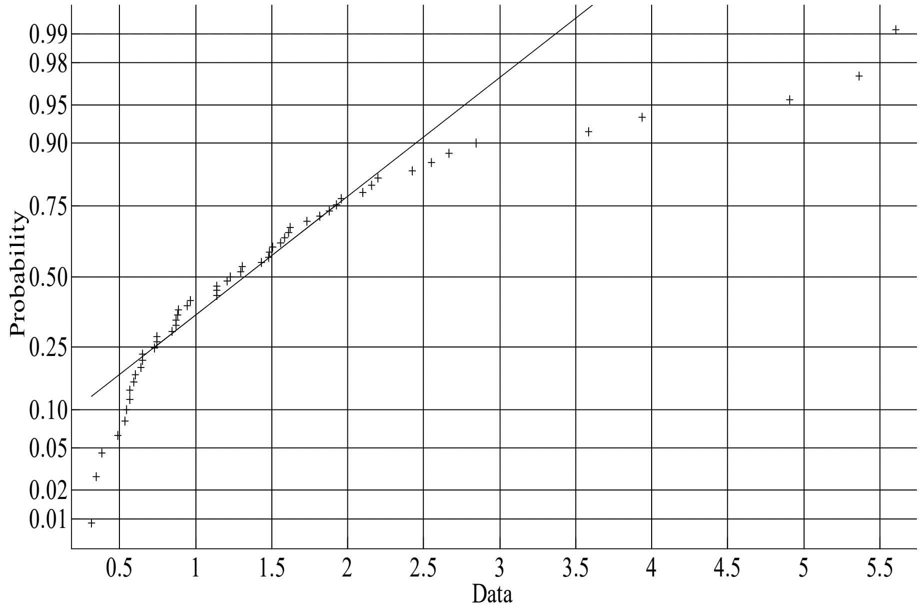

Figure 5-27 Normality plot for the NW catchment, $C_{ratio(s)}$ shown as 'Data' on the x axis.

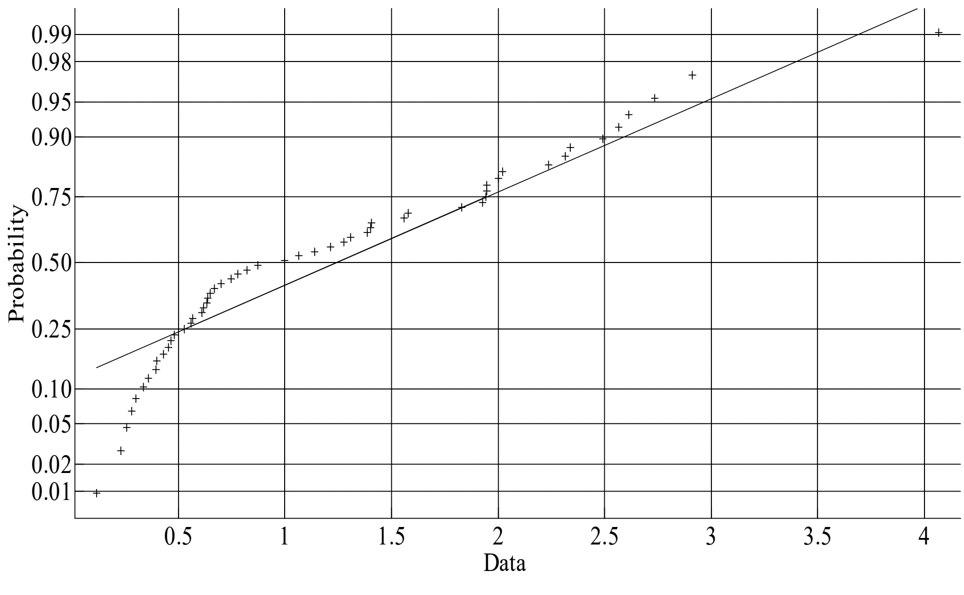

Figure 5-28 Normality plot for the RCW catchment, $C_{ratio(s)}$ shown as 'Data' on the x axis.

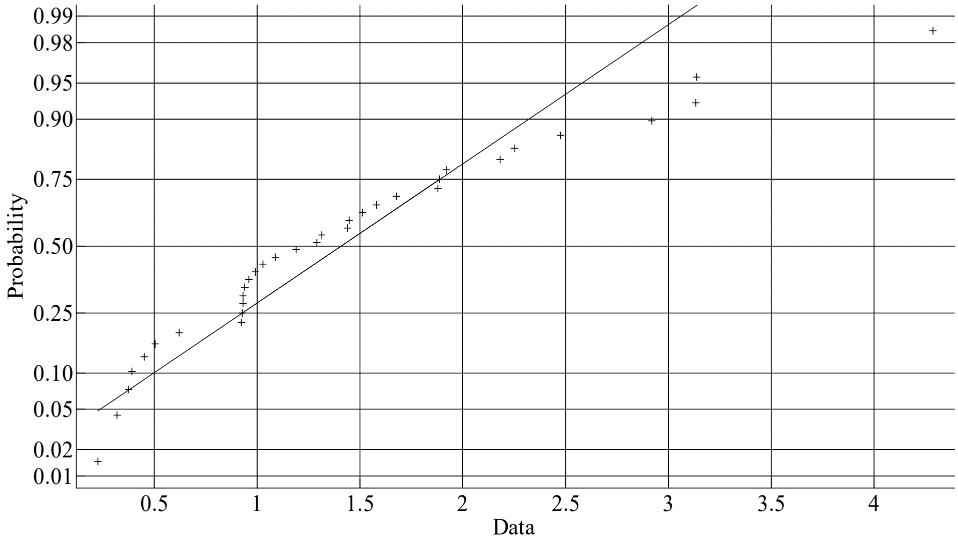

Figure 5-29 Normality plot for the RICH catchment, $C_{ratio(s)}$ shown as 'Data' on the x axis.

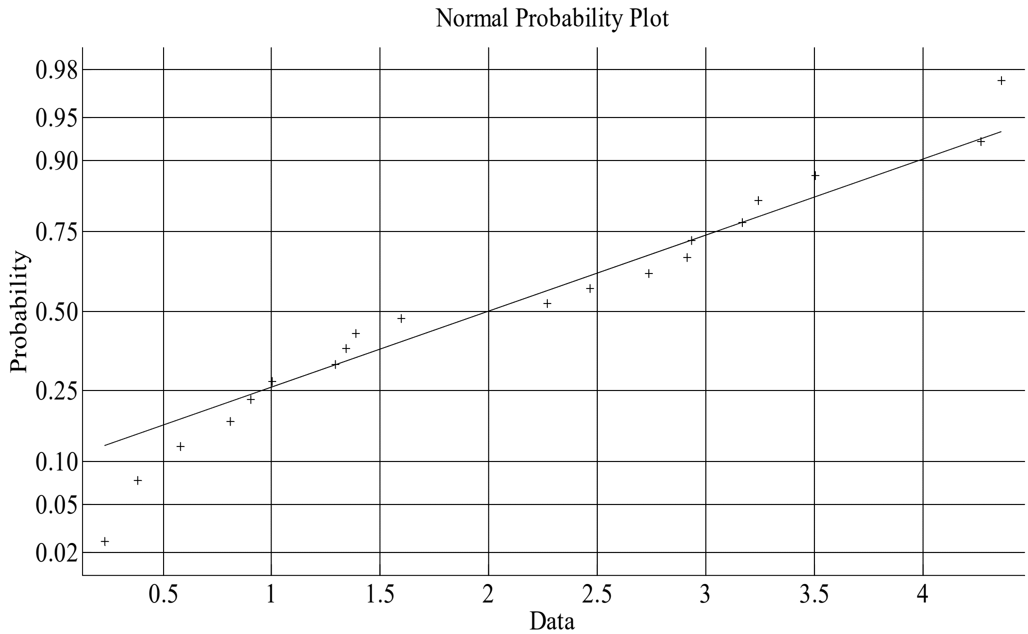

Figure 5-30 Normality plot for the SHEP catchment, $C_{ratio(s)}$ shown as 'Data' on the x axis.

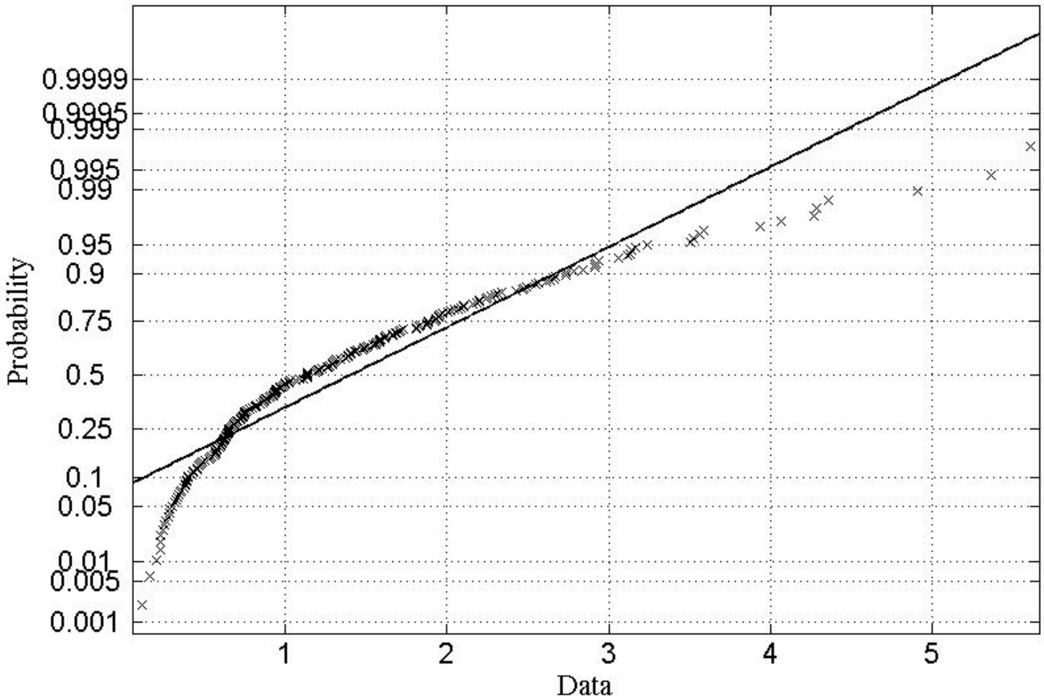

Figure 5-31 Normality plot for the combined catchments, $C_{ratio(s)}$ shown as 'Data' on the x axis.

A larger proportion of the model residuals fall in the negative range, this indicates that the model tends to under predict TSS EMC's. The model residuals visually show a departure from normality; they do not form a straight line. Histograms of $C_{\text{ratio(s)}}$ were plotted using Matlab's distribution fitting tool, bin sizes were calculated according to the Freedman Diaconsis rule (Equation 5-23):

Equation 5-23

$$Bin\ Size = 2 * \frac{IQR(x)}{\sqrt[3]{n}}$$

Where:

$Bin\ Size$ = number of bins

IQR = the Interquartile range of the data (x)

n = the number of observations.

Histograms of catchment $C_{\text{ratio(s)}}$ and all combined catchment $C_{\text{ratio(s)}}$ are presented in Figure 5-32.

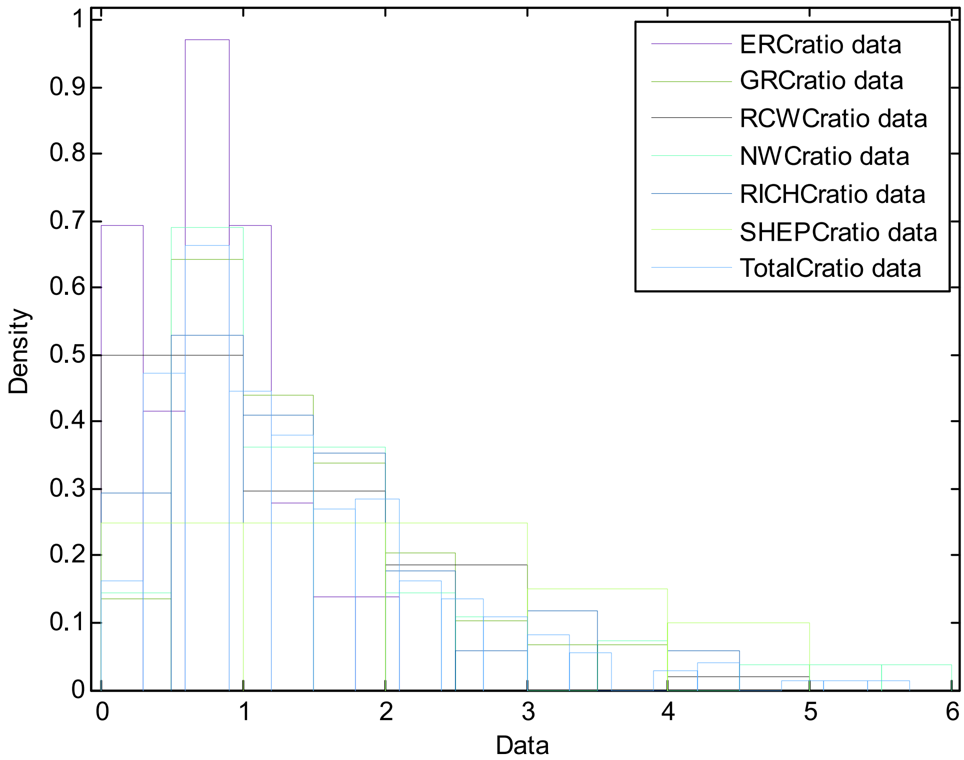

Figure 5-32 $C_{ratio(s)}$ Histograms of catchments ER, GR, RC, NW, RICH, SHEP and, all catchments combined

From visual inspection of histograms (Figure 5-32) it was apparent that the C_{ratio} values followed a heavily tailed distribution, therefore continuous probability distributions available in the Matlab Distribution Fitting tool were tested to determine the appropriate probability distribution to describe the $C_{ratio(s)}$ for each catchment and the combined catchment dataset respectively. The Matlab distribution fitting tool uses maximum likelihood estimation method to fit distributions to data (Myung, 2003). The Anderson-Darling statistic can be used in Matlab for statistical testing of whether data is drawn from a given probability distribution (Anderson and Darling, 1952). It is commonly used to test in situations where families of distributions are being tested, the lower the Anderson Darling 'goodness-of-fit' static (AD), the 'better' the selected probability distribution represents the data.

Table 5-14 Anderson Darling statistic for heavy tail distribution fits

Probability Distribution(s)	Anderson Darling Statistic (AD)					
	ER	GR	NW	RCW	RICH	SHEP
Normal	1.72	0.86	0.50	2.74	0.37	1.26
Log-normal	0.42	0.34	0.23	0.58	0.37	0.57
Weibull	0.93	1.01	0.44	1.803	1.01	1.00
Gamma	0.60	0.46	0.26	0.850	0.58	0.77
Loglogistic	0.81	0.68	0.26	0.613	0.33	0.92
Combined	0.78	0.51	0.36	1.16	0.48	0.84

Table 5-14 shows that the 'log-normal' distribution was correctly selected as the most appropriate distribution to represent all $C_{ratio(s)}$. In probability theory, a log-normal distribution is a continuous pdf of a random variable x whose logarithm is normally distributed. The probability density function y of the log normal distribution is given by:

Equation 5-24

$$y = f(x \mid \mu, \sigma) = \frac{1}{x\sigma\sqrt{2\pi}} e^{\frac{-(\ln x - \mu)^2}{2\sigma^2}}$$

Where:

μ = location parameter

σ = scale parameter

π = Pi (~3.142)

The two parameters μ and σ are not location and scale parameters for a lognormally distributed random variable x, they are location and scale parameters for the normally distributed logarithm ln(x).The lognormal distribution is applicable when the quantity of interest must be positive. The cumulative distribution function (cdf) of the standard normal distribution may be expressed as follows:

Equation 5-25

$$F(x|\mu,\sigma) = \frac{1}{\sigma\sqrt{2\pi}}\int_0^x \frac{e^{\frac{-(\ln(t)-\mu)^2}{2\sigma^2}}}{t}dt$$

Where:

μ = location parameter

σ = scale parameter

π = Pi (~3.142).

Matlab version R2013a (www.mathworks.com) can be used to compute confidence bounds associated with distribution pdf's and cdf's, these bounds represent lower and upper values of the associated interval, and define the width of the interval. The width of the interval indicates how uncertain a prediction is, the bounds represent a level of uncertainty. The level of uncertainty often used is 95%, thus the 95% prediction interval is computed. The interval indicated that there is a 95% chance that a prediction is contained within the lower and upper prediction bounds. Confidence intervals associated with model predictions are computed using this method in chapter 6 but are shown here for continuity.

Figures 5-32 to 5-38 show the histograms and fitted log-normal pdfs for catchments ER, GR, NW, RCW, RICH, SHEP and all catchment data combined respectively.

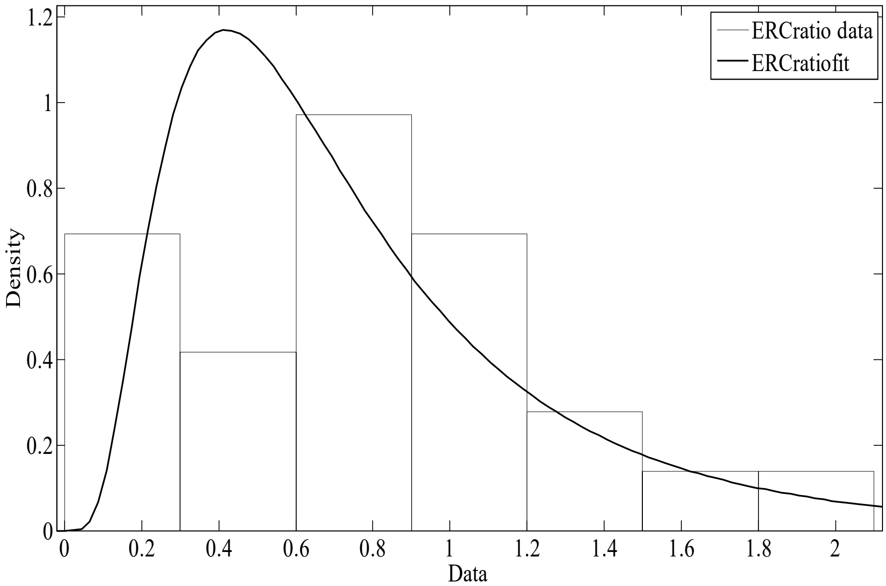

Figure 5-33 **Histogram and fitted log-normal distribution of $C_{ratio(s)}$ for the ER catchment**

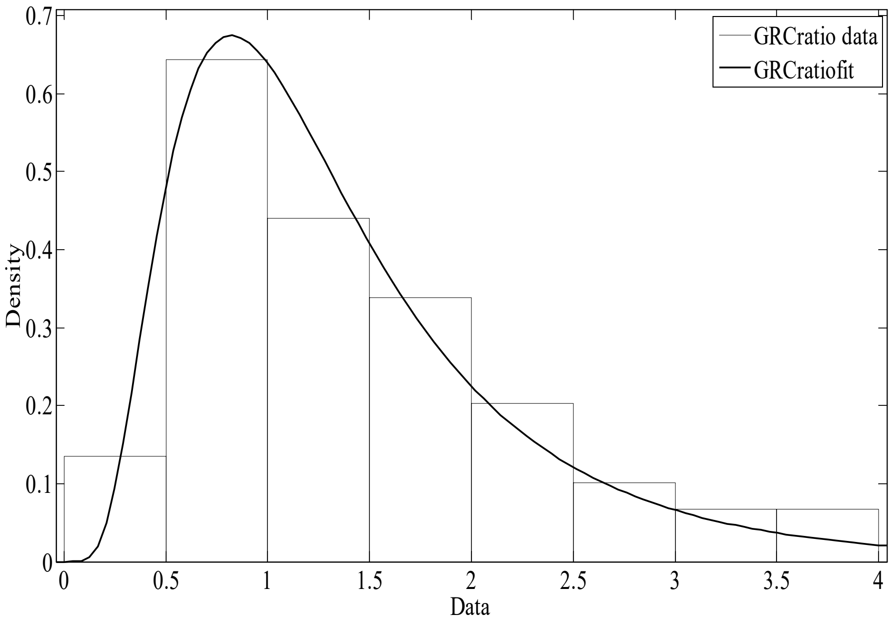

Figure 5-34 Histogram and fitted log-normal distribution of $C_{ratio(s)}$ for the GR catchment, $C_{ratio(s)}$ are shown as data on the x-axis.

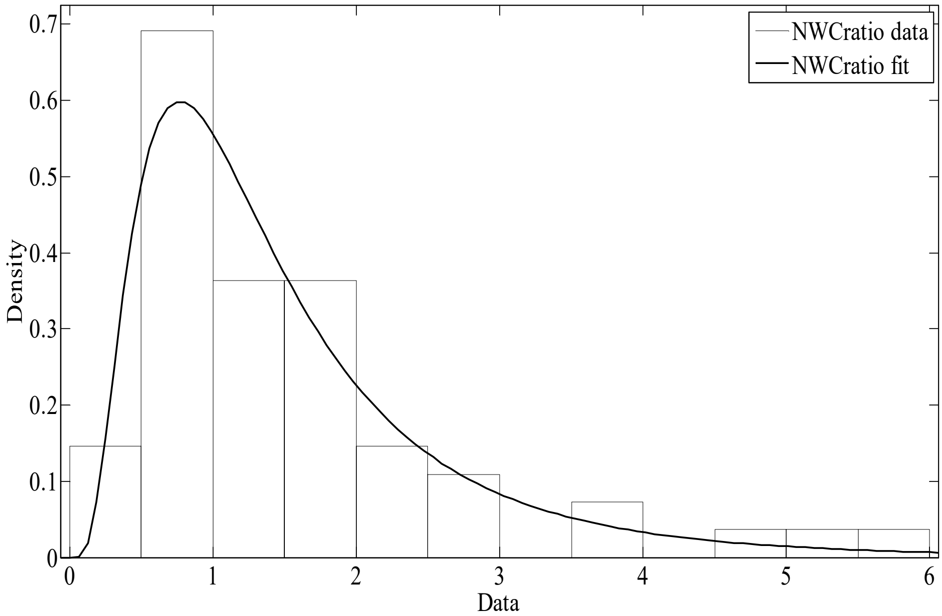

Figure 5-35 Histogram and fitted log-normal distribution of *C*$_{ratio(s)}$ for the NW catchment, $C_{ratio(s)}$ are shown as data on the x-axis.

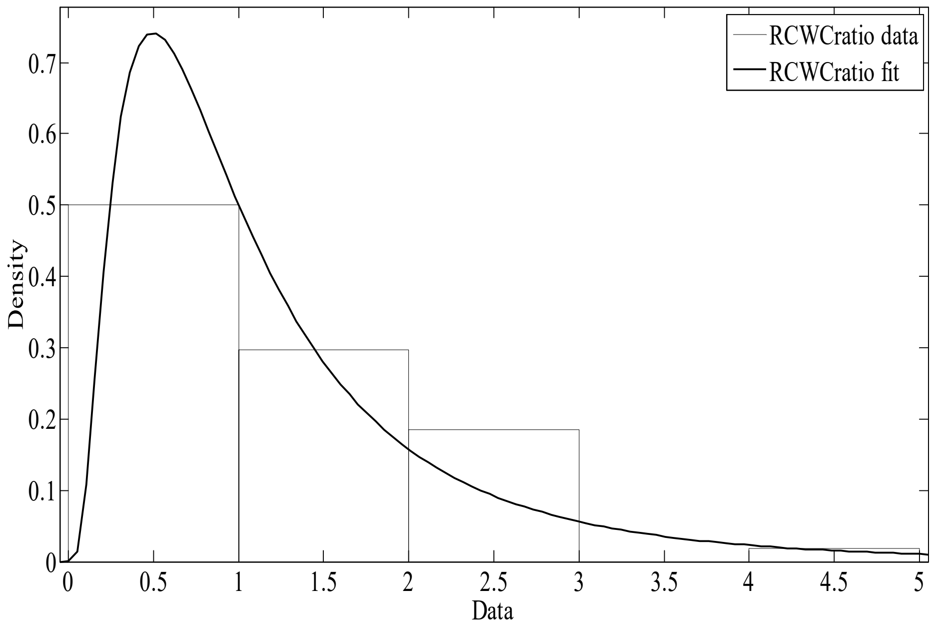

Figure 5-36 Histogram and fitted log-normal distribution of *C*$_{ratio(s)}$ for the RCW catchment, $C_{ratio(s)}$ are shown as data on the x-axis.

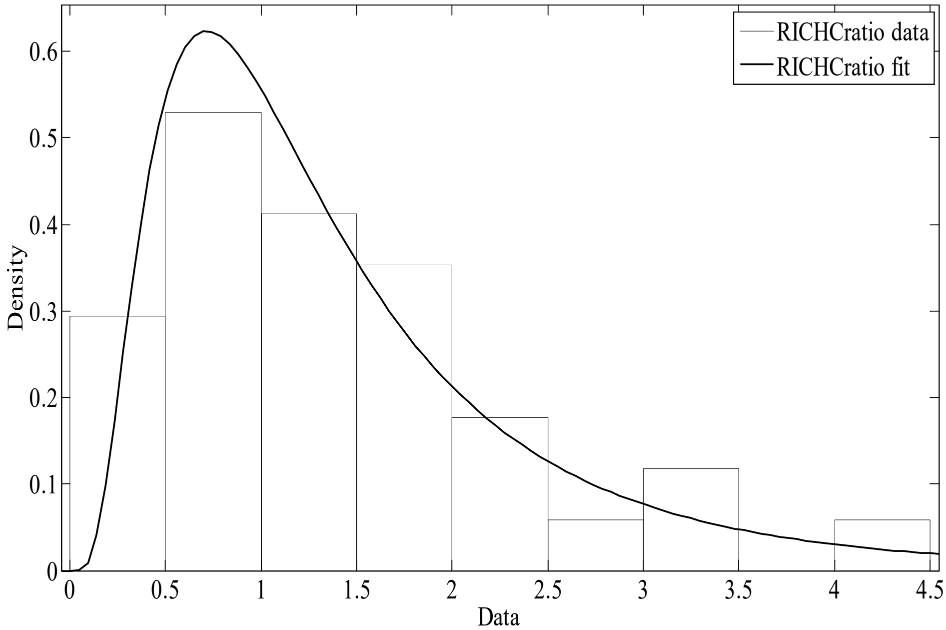

Figure 5-37 Histogram and fitted log-normal distribution of $C_{ratio(s)}$ for RICH catchment, $C_{ratio(s)}$ are shown as data on the x-axis.

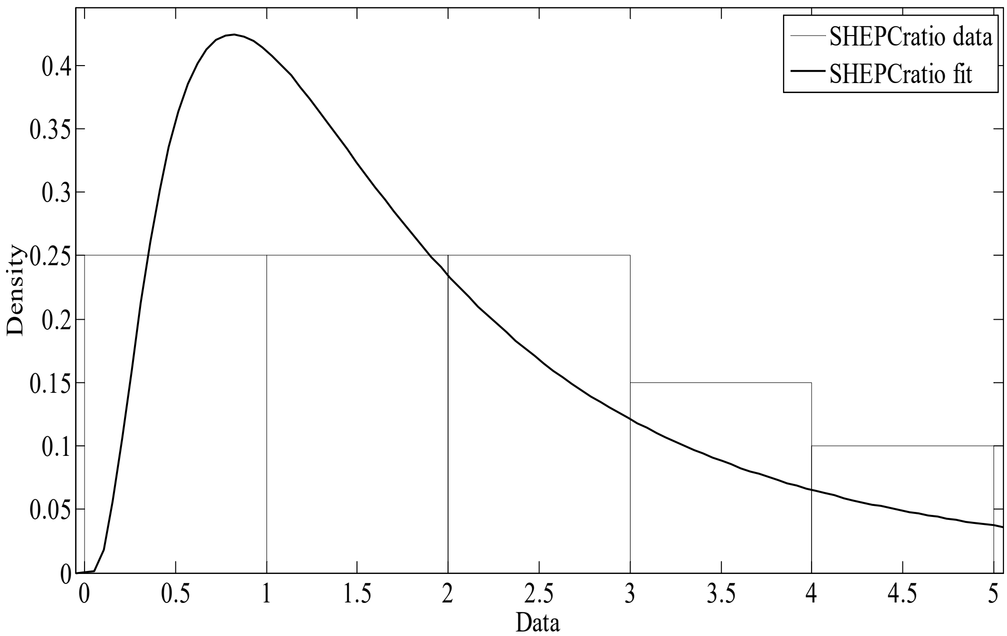

Figure 5-38 Histogram and fitted log-normal distribution of $C_{ratio(s)}$ for the SHEP catchment, $C_{ratio(s)}$ are shown as data on the x-axis.

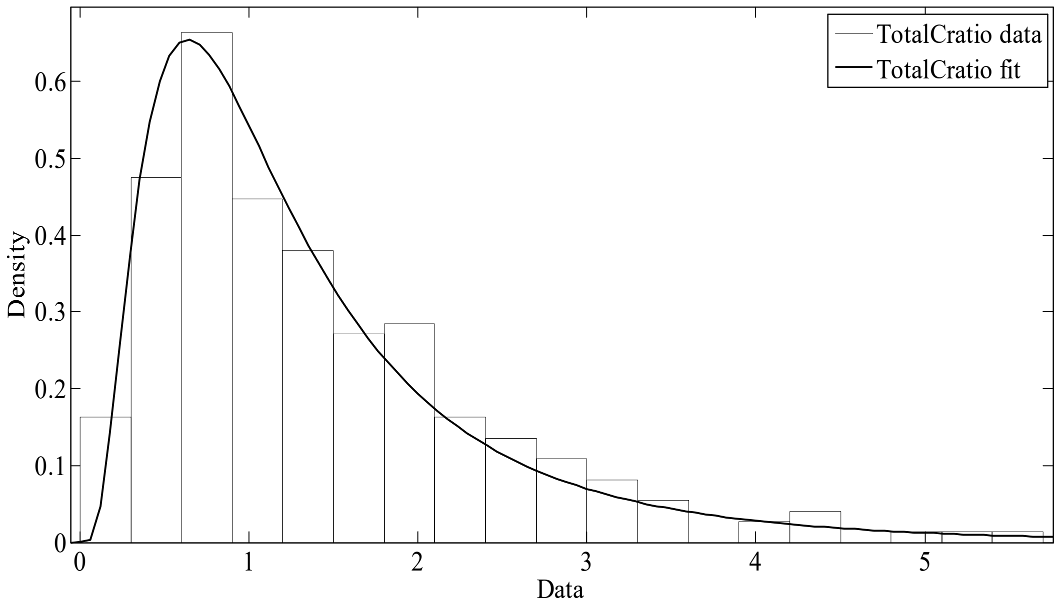

Figure 5-39 Log normal distributions of all combined catchment $C_{ratio(s)}$, shown as data on the x-axis.

The characteristics (mu and sigma) of each catchments C_{ratio} distribution and the pdf characteristics are presented in Table 5-15.

Table 5-15 C_{ratio} distribution fitting characteristics

Catchment	Sample size	$C_{ratio(s)}$ Mean	$C_{ratio(s)}$ Variance	Distribution fitting information: Fitted Distribution	Distribution parameters: *mu*	*u*	sigma
ER	24	0.79	0.34	Log-normal	-0.43	0.65	0.65
GR	60	1.41	0.86	Log-normal	0.16	1.17	0.60
NW	55	1.55	1.40	Log-normal	0.20	1.22	0.68
RCW	34	1.27	1.41	Log-normal	-0.07	0.93	0.79
RICH	54	1.43	1.43	Log-normal	0.15	1.16	0.69
SHEP	20	2.24	4.86	Log-normal	0.47	1.59	0.82

Combined	247	1.42	1.42	Log-normal	0.08	1.08	0.73

Following derivation of the C_{ratio} pdfs for each and the combined catchments respectively, Monte-Carlo sampling from the distributions attained can performed to quantify the uncertainty associated with model predictions (this method is presented in chapter 6).

The uncertainty procedure has been summarised below:

1. Calibrate model using methodology presented in section 5.2.1.1 on the catchment under analysis to obtain optimal parameter sets for C_0 and k. Alternatively use the parameters set derived in this work i.e. if catchment land-use is 'mixed residential', use ER parameter set.
2. Input chosen rainfall characteristics into model (T, ADWP and AGI5) and run model to generate prediction of TSS EMC's.
3. Trial uncertainty methodology presented in this chapter to 'estimate' uncertainty surrounding model prediction. The estimation of uncertainty through the use of confidence bounds is presented in chapter 6.

The application of this method is presented in chapter 6.

5.5 Discussion and conclusions

This aim of this chapter was to develop a new stochastic model capable of predicting storm water TSS EMC's. In section 5.1 'selection of model variables', a multivariate data analysis technique (PCA) was applied to TSS storm water quality data and possible corresponding climatic and rainfall variables to identify the explanatory variables which 'best' described variations in TSS EMC's. Whilst the PCA technique is reliable on the user's visual analysis of resulting bi-plots and is thus subject to human error when determining relationships between variables under analysis, the resulting bi-plot visual assessment suggested that variations in TSS EMC concentrations were best described by the rainfall characteristic variable AGI5.

The only climatic variable measured in this study was antecedent dry weather period (ADWP), whilst the PCA analysis 'did' suggest that this variable showed some capacity to describe catchment TSS EMC's, it did not appear to describe as much variation in TSS EMC's as AGI5, It is suggested in the literature that pollutant build-up is influenced by a wide array of factors such as the quantity of vehicular traffic in a catchment and catchment land use characteristics, however, with the literature suggesting that simple storm water quality models should conceptualize both build-up and wash-off processes and with no other climatic variables capable of describing the build-up phenomena available for study, the variable was included for further analysis prior to model development.

In Section 5.2 'model development' it was hypothesized that pollutant concentrations can be described by the exponential decay wash-off equation. The equation was mathematically derived to show a formulation capable of predicting TSS EMC's via the inclusion of three parameters; C_o; the initial pollutant concentration available to be washed; k, the rate at which this initial pollutant concentration is subsequently washed off and T; the duration of the event under analysis. It was hypothesized that the climatic variable ADWP could be used to estimate C_o and that AGI5 could be used to estimate k.

To investigate the use of different mathematical functions capable of predicting values of C_o and k, a statistical procedure in the form of regression equations and least squares fitting of explanatory variables was utilised within a specific calibration algorithm. The procedure showed that one of 15 statistical model formulations (model formulation 4B) predicted TSS EMC's more effectively on four of the six catchments analysed (ER, GR, RCW and RICH) with resulting RMSE values of 21.1, 35.1 34.2 and 60.4 mg/l obtained respectively. With regard to the two catchments where this model formulation was not the most effective at predicting TSS EMC's (NW and SHEP) it is apparent that all model formulations tended to perform poorly with mean RMSE values of the range 68.5 and 60.9 mg/l obtained respectively. This could be attributed to pollutant processes on these catchments poorly described by the exponential wash-off equation, this would concur with work by Bach (2010b), who noted that the catchment NW was subject to sewerage and storm water cross-connections, thus concentrations of TSS recorded on this catchment may be subject to inaccuracies.

Calibration of the model was considered successful on all catchments with E values all positive in the range of 0.18-0.91 this would suggest that the model structure is appropriate. Validation of the model was also deemed successful with E values in the positive range of 0.1-0.85. The E values attained for calibration and validation were distinctly variable across all catchments. The model performed well (E values above 0.5) when predicting TSS EMC's from the ER, RCW and SHEP catchments, all these catchments were classified as 'mixed residential' suggesting that these catchments resulting TSS EMC's are more heavily influenced by the explanatory variables described in this model (ADWP and AGI5),

It is difficult to comparatively evaluate the performance of the newly developed model against other studies due to the scarcity of information regarding model efficiencies in the literature, especially because most many of these studies have been performed on models which predict pollutant fluxes and loads (Kanso, Chebbo and Tassin, 2005). Furthermore, of the studies which have tested different build-up and wash-off models, few events were calibrated (Dembélé *et al.,* 2011). Regardless of the limited number of studies available for comparison, the performance of the model has been compared to the validation efficiencies presented in the literature and to the application of the model presented in Dembélé *et al.,* (2011) model efficiencies obtained in chapter 4 (Table 5-16).

Table 5-16 comparison of validation coefficients

Catchment evaluated	Validation Coefficients (E)			
	Dembélé *et al*., 2011	Dembélé *et al*., 2011 chapter 4	Dotto *et al*., 2010	Eq 5-20
ER	-	0.73	-	0.85
GR	-	-	0.07	0.32
NW	-	-	0.46	0.26
RCW	-	0.4	0.22	0.66
RICH	-	0.57	0.12	0.19
SHEP	-	0.79	0.06	0.67

ECULLY	0.78	-	-	-
CHASAEIU	0.91	-	-	-

The validation E values presented in Table 5-16 would suggest that the model shows an improvement on the build-up wash off approach previously evaluated on this data set (Dotto *et al.,* 2010), this could be attributed to the model accounting for rainfall explanatory variables rather than catchment characteristic to estimate build up. The model presented in Dembélé *et al.,* (2011) yielded higher E values on two of the six catchments evaluated; RICH and SHEP, lower E values on RCW and ER and showed negative E values (lower predictive capacity than the mean value of the data set) on catchments GR and NW. This variation in performance could be attributed to the fact that the model assumed two different distinct states which influence TSS EMC's. It should be noted that water quality model calibration is widely regarded as a challenging process and that very low model efficiency coefficients are commonly attained (often in the negative range) (Dotto *et al.*, 2010), thus the subsequently high model efficiency values presented in this chapter would suggest that the model does have a relatively high predictive capacity.

The newly developed TSS EMC model sensitivity to model inputs and parameter values has been evaluated by performing a GSA. The analysis showed the model is particularly sensitive to model parameter *c*, model inputs variables AGI5 and the duration of the event under observation, this would concur with work reported by (Lee *et al.*, 2011). The GSA suggested that model parameters *a* and *d* had little influence on the models predicted TSS EMC's in this build-up component, however it is noted that the GSA was performed by sampling uniform input distribution ranges obtained the recorded field data. To improve this analysis, input distributions could be cited from the literature. Due to the structure of the function for C_o, with decreasing values of variable ADWP, predicted TSS EMC's would become increasingly sensitive to parameter b. In the wash-off component of the model, represented by *k*, predicted TSS EMC's were most sensitive to changes in parameter d, model sensitivity to this parameter increases as the value of d decreases. The model was not sensitive to parameters d and b, it is therefore assumed that these parameters could be fixed.

The model assumes that TSS EMC's are limited to the amount of pollutant available to be washed off, represented by model component C_o. This initial component of the model assumes that there is no pollutant available to be washed off, thus ADWP = 0. This is the main weakness of the model in that its temporal resolution is on the event scale, thus it functions irrespective of accumulated pollutant levels that may remain on a catchment from the previous event. For example, if the previous event to the one under analysis had a significantly high build up period (ADWP) then the resulting potential for large pollutant loads to be washed off during this event would be high. If only a small fraction of pollutant is washed off, the capacity for pollutants to be washed off in the event under analysis would be high, regardless of the ADWP. The consequence of this is that if the model under analysis had a small ADWP, then the model would assume the amount available to be washed off would be low, when in fact this could be significantly large. It has been suggested that the amount of pollutant available to be washed off during a rainfall event reaches equilibrium at approximately 9 days, thus events with a higher ADWP would be less susceptible to errors caused by this model assumption (Deletic, 2005).

The latter parts of this chapter described the development of a methodology for estimating uncertainty in the proposed model. As discussed in chapters 1 and 2, there is an inherent uncertainty associated with water quality predictions due to the inherent variability of water quality processes; specifically, build-up and wash-off (Daly, 2014). To account for this natural variability, a Monte Carlo simulation approach utilizing residual model errors derived during calibration was utilized to produce uncertainty bounds associated with model prediction. This approach assumed that all the contributing sources of uncertainty are captured by the model residuals errors, however, it is highly unlikely that there were no data collection errors in the observed TSS data set. The mean residual error across all six catchments was 7.9 mg/l in the positive range, this would suggest that the model under predicts TSS EMC's, this again could be attributed to the model's inability to account for accumulated loads.

Following standardization of model residuals, $C_{ratio(s)}$ were obtained for each catchment and resultant distribution fitting data presented in table 5-15. The only catchments categorized as 'commercial and industrial' usage showed the least C_{ratio} variance; ER and GR 0.34 and 0.86 respectively. All other catchments -

categorized as 'residential' - showed C_{ratio} variances in the range 1.40 – 4.86, this could indicate that modelling uncertainties are more likely in areas in residential areas where anthropogenic activity takes place. Based on the results presented in Table 5-2 - Table 5-7, model formulation 4B was judged to be the most effective at describing variations in TSS EMC's across all catchments, however, the SHEP catchments most effective formulation was 2C, the only model with differing components for both build-up and wash-off, this could explain why such a large C_{ratio} variance (4.86) was obtained for this particular catchment. The variance could also be attributed to a small number of events being monitored on this catchment and subsequent lack of calibration data with which to capture the variation of TSS EMC's within this catchment.

Chapter 4 discussed the difficulty of transferring statistical stormwater models on catchments other than where they were originally calibrated. In this chapter, a new TSS EMC model has been developed which predicts TSS EMC's for the catchments on which it was developed. To evaluate the transferability of this model, chapter 6 applies the model to the UK catchment data set presented in chapter 3.

Chapter 6. Model Application and Transferability

Chapter 4 discussed the difficulty of transferring simple storm water models to catchments other than where they were originally calibrated. In chapter 5, a model was developed which used explanatory climatic and rainfall event variables to predict TSS EMC's and an associated methodology which could be used to quantify the levels of uncertainty model prediction. The aim of this chapter is to study the transferability potential of the model to a catchment other than where it was originally developed, more specifically, the chapter aims to:

1. Use a complex deterministic model to generate a synthetic water quality data set for one of the UK catchments presented in chapter 3.
2. Calibrate and validate the newly developed model presented in chapter 5 to the synthetic water quality catchment data set generated in (1).
3. Validate the model using the observed water quality catchment data presented in chapter 3.
   - Apply the Factor ratio uncertainty method developed in chapter 5.
4. Show how the model could be utilized in a practical context to aid solution design within the ICM procedure.

There are risks and problems associated with the approach presented in this chapter, in that the model developed in chapter 5 was developed using data collected from a separate stormwater collection system. The data used to test in chapter 3 were collected from combined stormwater and wastewater systems, therefore any objective evaluation of the model's transferability could be considered 'weak'. In respect of this weakness, the work in this chapter is focussed on presenting how the model and methodology presented in chapter 5 could be utilised to aid the solution design component of the ICM procedure; by using calibrated complex deterministic models as 'surrogates' for simpler models with reduced computational costs.

6.1 Development of a Synthetic Water Quality Data Set

In chapter 5, 247 storm water quality events over a range of climatic and rainfall conditions were monitored on 6 different catchments to develop a simple TSS

EMC model with uncertainty quantification capabilities. It is hypothesized that the 'complex' deterministic water quality model InfoWorks CS presented in chapter 3 could be used to generate a synthetic water quality data set with which the model could be calibrated, subsequently, the model could be verified using a small number of observed water quality data available for the respective catchment under investigation, similar approaches to the use of complex models as 'surrogates' to develop data sets with which simple models can be calibrated are presented in the literature (Freni et al., 2008).

The InfoWorks CS models of the four sewer network catchments presented in chapter 3 and this chapter were assumed to sufficiently represent reality; their model, build and verification checked against regulatory and best practice modelling practices presented in chapter 2 by the EA and subsequently approved for the development of ICM solutions in AMP3. As this chapter's focus is on the possible application of the model within the ICM procedure, its application has been performed with on one catchment and it's respective InfoWorks CS sewer model; the Denton catchment.

The synthetic water quality data set was created via the built-in InfoWorks CS UK rainfall generator. The model can be being used to create synthetic rainfall events, each event could then be characterized to obtain the necessary event model input variables; antecedent dry weather period (ADWP), rainfall event duration (T) and rainfall event average intensity (AGI5). The pre-calibrated catchment response to these synthetic rainfall events (InfoWorks CS predictions of TSS concentrations at a chosen CSO) were then analyzed to obtain respective TSS EMC's for each event.

Generation of Synthetic Rainfall Events

The software InfoWorks CS (version 12.5) (www.innovyze.com) has a built-in rainfall generator which allows users to generate synthetic rainfall events. The synthetic events generated are based on research by the UK meteorological office, whereby statistical rainfall relationships have been derived from long term rainfall records across the UK. These statistical relationships allow users to generate a representative rainfall event for any location in the UK, duration and return period. Further information on this process can be found in The Wallingford

Procedure (DoE/NWC, 1982) and in the Flood Estimation Handbook (FEH) (Centre for Ecology & Hydrology (formerly the Institute of Hydrology), 1999).

Rainfall Generator Parameters

To create synthetic rainfall events time series events within InfoWorks CS, several parameters (rainfall event, catchment and catchment initial condition) must first be set within the rainfall generator model (Innovyze, 2011). These parameters are:

- Rainfall event parameters:
    - Return period.
    - Duration.
    - Profile.
    - Multiplication factor.
- Catchment parameters;
    - 5-year 1-hour rainfall (20)
    - Rainfall ratio (0.4)
    - Catchment area (1151 Ha)
- Initial conditions Parameters
    - Urban catchment wetness index (UCWI) (80)
    - Antecedent Depth (10mm)
    - Wetness Index (0)
    - Evaporation (mm/day)

In the context of this study, the return period is an estimate used to indicate the likelihood of a rainfall event. These likelihoods are derived from historical rainfall records (HR Wallingford, 1981). They are often used in risk-based analyses to design of solutions which are able to 'withstand' an event of certain statistical likelihood. They assume that the probability of an event is independent of past events and does not vary over time.

Equation 6-1

$$\frac{n+1}{m} = Return\ period$$

Where

n = the number of years of data

m = the number of occurrences of the event under study.

Return periods are also expressed as 'expected frequencies', this expression of the return period is the inverse of the expected number of occurrences in a year i.e. a 10-year flood has a 10% chance of being exceeded in one year.

In the InfoWorks CS model, the return period (years) indicates the period (years), between rainfall events of greater or the same intensity than the storm being generated. Because the winter and summer rainfall profiles are used for specific types of analyses, the return period must be between 1 and 100 years, if the synthetic rainfall profile is selected, rainfall events of less than 1-year return period can be defined. For example, a 1 in 1-week rainfall event can be defined as a '52 in 1-year' rainfall event, thus the return period is defined in the software as -52. Furthermore, a '1 in 6-week' rainfall event can be defined as a '2 in 1' year rainfall event, thus the return period is defined as -2. To calibrate the model to 'realistic' conditions, both short and long-term return periods are required, thus multiple 'summer' and 'synthetic' profiles were utilized to create rainfall events.

Rainfall Event Duration and Profile

The duration of the rainfall event must be defined within the rainfall generator. The rainfall duration used is often dependent on the size of the catchment; with short storms having higher peak intensities and long storms having a larger total rainfall depth (Robson and Reed, 1999). A summer, winter or synthetic profile must be defined in the rainfall generator. This profile defines how high the peak intensities are for a given rainfall depth, the Wallingford procedure recommends using the '50^{th} percentile summer profile; high peak intensities for urban areas, thus these were selected for rainfall events over the 1-year return period.

Multiplying factor

The multiplying factor allows for a percentage-based increase of design rainfall events. This parameter was not utilized in this study and so a value of 1 was used for all generated rainfall events.

Catchment Parameters

The catchment parameters specify the initial conditions associated with the catchment.

5-year 1-hour rainfall

This is the rainfall depth (mm) for a 5-year return period rainfall event of 1-hour duration. Reference 5-year 1-hour values can be obtained with respect to the catchments location (Centre for Ecology & Hydrology (formerly the Institute of Hydrology), 1999).

Rainfall ratio

The rainfall ratio is the ratio of rainfall depths for a 5-year return period rainfall event of 1-hour duration and a 5-year return period rainfall event of 2 days duration. Typical values across the UK are in the range of 0.12 to 0.46. Ratios can be obtained can be obtained with respect to the catchments location (Centre for Ecology & Hydrology (formerly the Institute of Hydrology), 1999).

Catchment Area

This rainfall generator input parameter represents the total catchment area of the drainage system. This value determines the area reduction factor, a factor which considers the reduction in total rainfall intensity as the storm passes over a catchment, it accounts for the spatial variability of rainfall events (Centre for Ecology & Hydrology (formerly the Institute of Hydrology), 1999).

Series

If using ‘synthetic’ rainfall event profiles, the respective catchments yearly ratio (YR) can be calculated by:

Equation 6-2

$$YR = \left(\frac{SAAR}{M5-60}\right) * R$$

Where:

SAAR is the annual average rainfall (mm)

M5-60 = the 5-year 60-minute rainfall event (mm)

R = the rainfall ratio (-).

InfoWorks CS allows users to choose a different ration for 'east' and 'west' locations, the YR closest to the predefined east (15.9) and west values (12.5) is then chosen. These ratios have little effect on storms over a 1-year return period (Centre for Ecology & Hydrology (formerly the Institute of Hydrology), 1999).

The initial event conditions specify the initial conditions associated with the moisture content of the catchment surface before a storm event begins.

The Urban Catchment Wetness Index

The Urban Catchment Wetness index defines the antecedent wetness of the catchment for the runoff model; this was set to 0.8, the default parameter defined within the model (Centre for Ecology & Hydrology (formerly the Institute of Hydrology), 1999).

Antecedent Depth

The antecedent depth (quantity of rainfall (mm) to have fallen an hour prior to the storm under analysis) was set to 10mm (worst case scenario) to ensure that any initial loss volume is filled before a storm commences (Centre for Ecology & Hydrology (formerly the Institute of Hydrology), 1999).

Wetness Index and evaporation

The wetness index defines the catchment wetness (dry, average or wet) for use within the run-off model. The evaporation define the rate of evaporation from the catchment per day (mm/day), it was set to the corresponding model default parameter described in the description of the Denton catchment (Chapter 3) (Centre for Ecology & Hydrology (formerly the Institute of Hydrology), 1999).

Selection of rainfall events

30 events were selected for synthetic generation. As discussed in chapter 4, ADWP's are assumed to influence the amount of pollutant 'build-up' and thus influence the quantity of TSS on the catchment surface available for wash off into

the combined sewer system. The InfoWorks CS model assumes that quantities of TSS on the catchment surface reach equilibrium at ADWP's of 9 days (Innovyze, 2011). Synthetic rainfall events were created for simulation on the catchment at ADWP periods of 0.2; 1; 2.5 and 9 to simulate a 'realistic' range of build-up conditions. In respect of the experimental values presented in the Monash water quality monitoring campaign presented in chapter 4, rainfall events durations were created at following intervals; 30, 60, 120 and 720 minutes for return periods of -52, -26, -13, -2 and 5 respectively. A summary of synthetic rainfall characteristics and possible ADWP's are presented in Table 6-1.

Table 6-1 Summary of climatic and rainfall event characteristic used to generate synthetic data set.

ADWP	Rainfall Durations	Return Periods
0.2	30	-52
1	60	-26
2.5	120	-13
5	720	-2
9	-	5

If all possible rainfall durations at the varying return periods were generated, it would require the simulation and corresponding analysis (calculation of TSS EMC's for each of event from high temporal resolution data) of 96 events. To simplify this procedure and minimise the calibration data set whilst also capturing the range of possible ADWP and rainfall event conditions, all possible deviations of rainfall events at corresponding ADWP's were created and 5 events selected at random 'with non-replacement' within MATLAB; none replacement meant that no event of the same characteristics was used twice to create the data set. As previously discussed, 30 events were created, 5 of these events were selected at random for model validation. The selected event conditions used for synthetic data generation are presented in Table 6-2 (events randomly selected for validation are greyed out).

Table 6-2 Summary of synthetic events used to generate synthetic data set. *Events reserved for validation are presented in grey.*

ADWP 0.2 (Days)		ADWP 1 (Days)		ADWP 2 (Days)		ADWP 5 (Days)		ADWP 9 (Days)	
RP	DUR (mins)	RP	DUR (mins)	RP	DUR (mins)	RP	DUR (mins)	RP	DUR (mins)
-26	60	-13	30	-13	30	-13	120	-13	120
-2	30	-13	60	-26	30	-2	60	-2	30
-52	30	-26	120	-2	720	-52	120	-2	60
-52	120	-2	720	-52	30	1	60	-52	30
1	120	-52	30	-52	60	5	30	1	720
5	30	5	720	5	30	5	120	5	30

6.2 Generation of Synthetic TSS EMC's

The catchment selected for analysis was Denton (catchment D), information on the network model build for this catchment is presented in chapter 3. Spill water quality results for the CSO prior to the WWTW (Figure 3-2, CSO 15) was selected at random for analysis.

Because the InfoWorks CS model representation is that of a combined system, to generate values of storm water TSS EMC's without contributions from domestic and industrial wastewaters, the wastewater profile used to provide inputs of wastewater within the model was turned off.

The InfoWorks CS software provides a complex representation of water quality processes within catchment sewer systems, this includes complex 'in-pipe' sediment behaviour which influence the concentrations of TSS spilled through a CSO. To account for the possibility that TSS concentrations could be significantly influenced by these behaviours, and the models predicted concentrations of TSS spilled out through the CSO under observation were homogenous for the rainfall simulation and subsequent ADWP being utilised, a stabilization procedure was created. To perform stabilization, ADWP's were spliced into a continuous time-series; whereby the ADWP was repeated until TSS concentrations spilled out through the CSO under analysis reached equilibrium. Once equilibrium was achieved, time-series data of TSS concentrations were exported to MATLAB for calculation of each respective event TSS EMC calculation. An example of this stabilization procedure is presented in Figure 6-1.

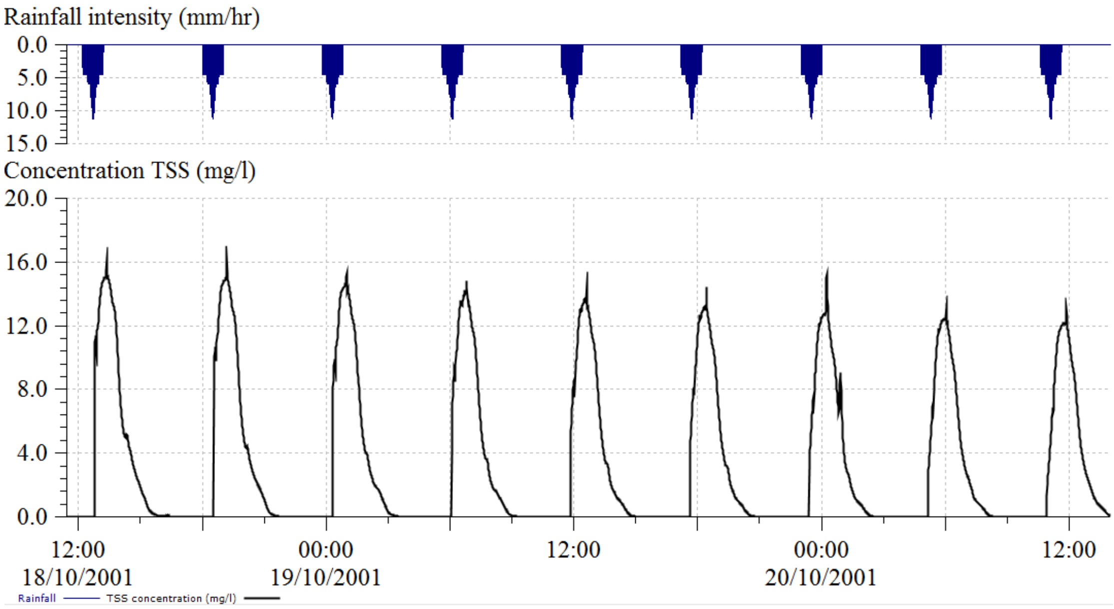

Figure 6-1 Plot of time series TSS concentration during simulation ADWP (0.2) *for event* RP(-26) DUR(60), convergence of stable concentrations can be seen in the last two CSO spill events for which equal values of TSS EMC were obtained.

Following calculation of TSS EMC's for each respective simulation, the newly developed model was calibrated to the synthetic TSS EMC data set via implementation of the calibration algorithm presented in section 5.2.1.1. Model calibration and validation results are presented in Figure 6-2 and Figure 6-3 respectively.

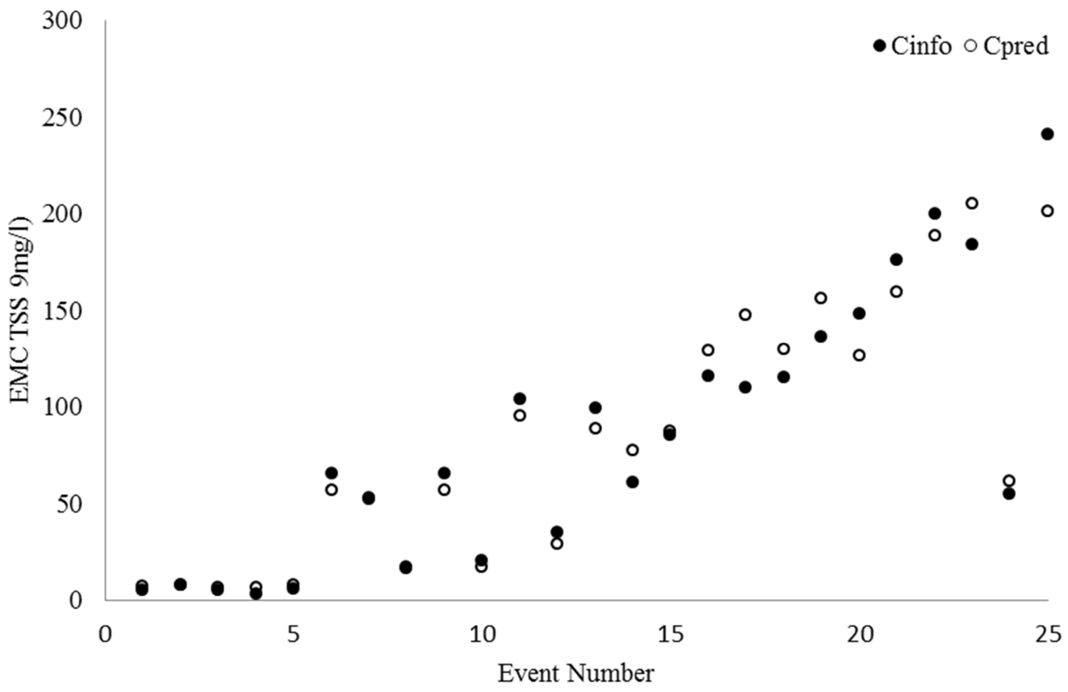

Figure 6-2 Calibration plot for Denton catchment showing TSS EMC's generated via InfoWorks CS (Cinfo) and calibrated model TSS EMC predictions (Cpred).

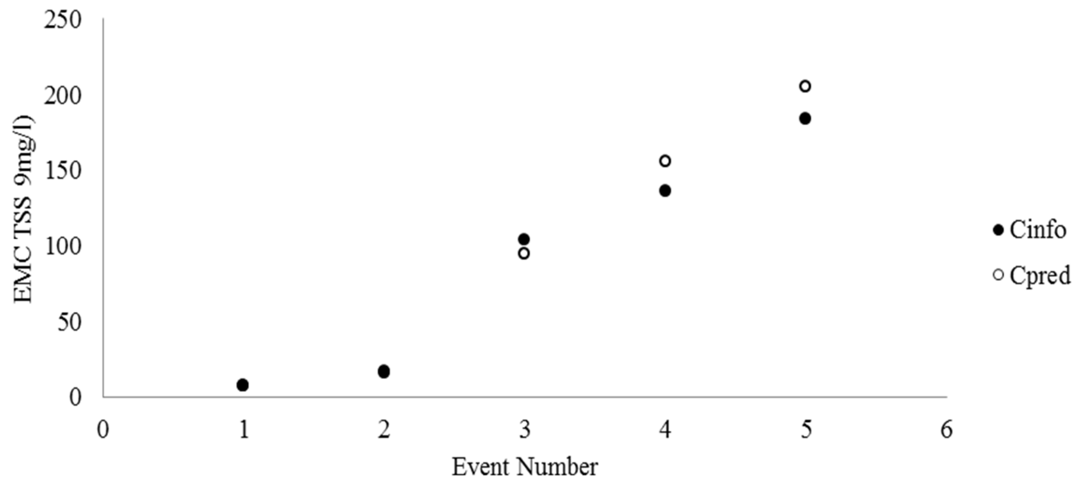

Figure 6-3 Validation plot for Denton catchment showing calibrated model TSS EMC predictions *vs InfoWorks CS* generated TSS EMC's.

Model parameter values and respective Nash-Sutcliffe coefficients (E) for both calibration and validation to the InfoWorks CS synthetic data set are presented in Table 6-3.

Table 6-3 Denton Model Parameter, Calibration and Validation Nash-Sutcliffe efficiencies

	Model Parameters				Calibration		Validation	
	a	b	c	d	No of events	Calibration (E)	No of events	Validation (E)
Denton	96.1	1.3	0.0048	-0.74	25	0.94	5	0.96

6.3 Application of Factor-Ratio Uncertainty Method

In this section, the 'factor-ratio' method presented in section 5.4 has been applied to quantify the uncertainty associated with model predictions. In chapter 5, pdf's were generated for the $C_{ratio(s)}$ of all catchments analysed, the 'combined' log-normal PDF has been utilised within the factor-ratio method to quantify the newly developed models uncertainty estimation on the Denton validation data; at the lower and upper 95% confidence intervals (Figure 6-4).

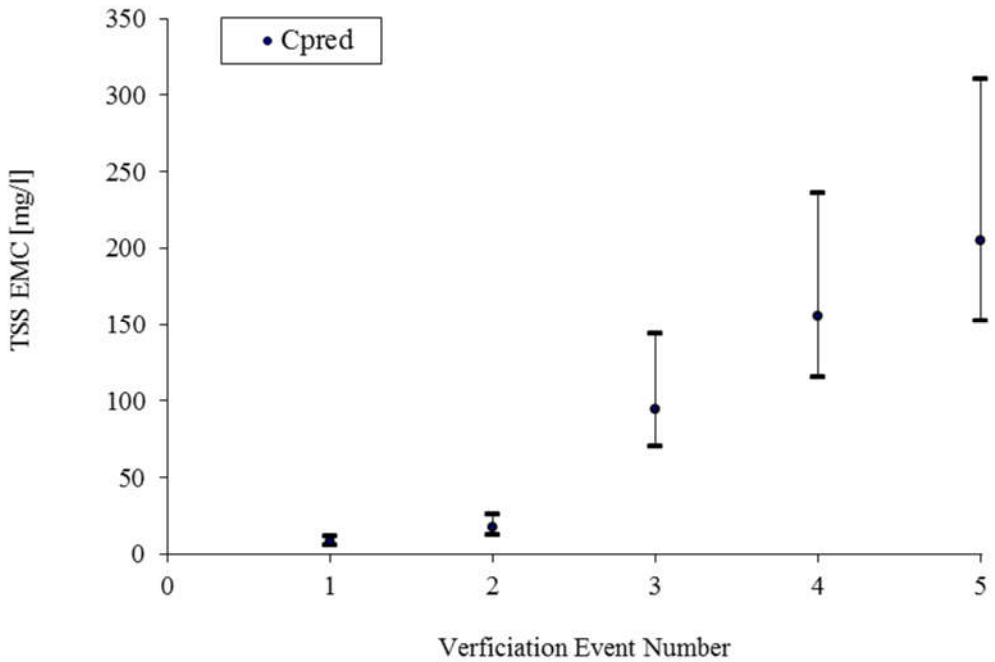

Figure 6-4 Uncertainty bounds calculated at the lower and upper 95% confidence interval for model prediction on the Denton catchment.

Figure 6-5 shows that the model's prediction becomes increasingly uncertain when predicting higher values of TSS EMC's, i.e. for validation event 6, the new model predicts a TSS EMC of 204 (mg/l), lower and upper 95% confidence intervals in the range 152 – 236 (mg/l) respectively.

Application of Model to observed values

Chapter 3 of this study presented water quality data for two observed storms on the Denton catchment, on receipt of this data set, no climatic variables were provided. To further validate the new model on this catchment (past the use of the synthetic water quality data set) ADWP's for these events were extracted from long-term rain-gauge data provided by United Utilities. Model parameter values derived from the initial model calibration in section 5.2.1.1, Table 5-2 Model inputs variable, models EMC predictions and associated uncertainty bands are presented in Table 6-4.

Table 6-4 Model inputs for the two observed events recorded at CSO 15 within the Denton catchment.

	Rainfall event characteristics			TSS EMC's (mg/l)			95% Confidence Intervals	
Rainfall Event	ADWP (days)	AGI5 (mm/hr)	T (mins)	Observed	Predicted	Variance	Upper	Lower
1	3.4	1.1	1650	30.4	24.3	6.21	47.6	23.4
2	2.3	2.9	132	141.3	98.0	43.3	146.7	70.3

The model under predicts observed values of TSS during both rainfall event 1 and 2, the observed values do fall within the 95% confidence limits calculated by the factor-uncertainty method.

6.4 Discussion and conclusions

The aim of this chapter was to investigate the transferability of the simple TSS EMC model developed in chapter 5, this was achieved through application of the model and associated uncertainty methodology applied to the Denton catchment and presented in chapter 3.

Due to data scarcity, calibration of the model was achieved by use of a synthetic water quality set generated by a previously calibrated and verified complex deterministic model. There are risks and weaknesses associated with this approach in that the new models predictive capacity is inherently linked to the complex models capacity to describe variations in TSS concentrations, an 'ideal' scenario would be to calibrate the model to a large number of water quality events which captured the maximum variation in catchment TSS catchment concentrations over a wide range of climatic and rainfall characteristics, however, in reality, water monitoring campaigns are expensive, climatic and rainfall conditions are uncertain and access to high quality water quality data is limited. Figure 6-4 shows the range of TSS EMC's captured by the synthetic calibration data set (4 – 249 (mg/l), this shows the advantage of using the synthetic calibration technique; a very few number of synthetic events (25) can be generated which captures a catchment response over a wide range of climatic and rainfall conditions.

Model calibration yielded high Nash-Sutcliffe values of 0.94 and 0.96 respectively; this highlights the ability of the model to 'mimic' the water quality description techniques used within InfoWorks CS model. According to model calibration, the optimal parameter set derived for the Denton catchment (excluding parameter d; -0.75) was within the range of the parameter sets obtained from calibration of the six Australian catchments in chapter 5, consequently, this larger value of parameter d reflected that model's predictions presented in this chapter were increasingly influenced by the wash-off component of the model.

Following model validation to the synthetic validation data set, further validation of the model was performed on the observed TSS EMC data presented in chapter 3. Whilst this data set consisted of just two monitored water quality events, following application of the Factor Ratio uncertainty method presented in chapter 5, the observed values of TSS EMC's for both rainfall events fell within the upper and lower 95% confidence intervals of the model for both events (Table 6-4). Application of this method involved sampling from the C_{ratio} pdf presented in chapter 5 for the 'combined' catchment data set. With random fluctuations likely to vary across catchments, it is recommended that recalculation of C_{ratio} pdf's for the catchment under observation be calculated; this approach is limited to the availability of observed catchment water quality data. The model was calibrated on a synthetic water quality data generated from a complex mode, the construction of the synthetic rainfall data as model inputs has little scientific foundation, therefore it is not possible to objectively evaluate the model's transferability. This chapter does however illustrate how the model and methodology developed in this work could be applied to simplify the solution design process within the ICM approach.

Chapter 7. Conclusions and Further work

The overarching aim of this work was to investigate and evaluate the potential of less computationally demanding water quality modelling technique to represent a specific component of the ICM process. Following an introduction to the urban drainage system and a review of the models used to support the ICM process (chapter 2); several specific research objectives regarding the development of a simple water quality modelling approach capable of providing a balance between model result accuracy and computational efficiency were presented. To meet these objectives, catchment water quality data sets collected across ten different catchments in the UK and Australia were analysed; a new stochastic water quality model and uncertainty methodology was developed from the analyses. After completing the study, the following conclusions have been made.

7.1 Evaluating the Use of Simple Water Quality Models within Integrated Catchment Models

Simple water quality models are less detailed representations of reality and operate at reduced temporal and spatial scales. This simplification means that these models require reduced computation cost when compared to their complex counterparts. Reduced model run times allows these models to be used more readily in scenario analyses and uncertainty assessment techniques. With the accuracy of complex water quality models often questioned within the literature, and a need to explicitly quantify the uncertainty associated with water quality predictions, chapter 4 aimed to establish whether there was a potential for simple water quality models to be used within the ICM approach.

EMC's are an inherently simplified approach to water quality modelling as the temporal variability of a spill event cannot be considered using a mean concentration value. Within respect to the integrated catchment modelling approach, EMC models may be used to provide inputs to river impact water quality models; the use of empirically based EMC's is a common alternative to deterministic hydrodynamic water quality modelling approaches when predicting the impact of combined sewer spills on receiving waters. The chapter utilised a previously conducted ICM study in the UK to explore the significance of the representation of dynamic pollution events as mean values within an ICM study.

As simple water quality models generate water quality descriptions at reduced temporal scales, it was necessary to quantify what the impact of such a reduction would have on overall ICM accuracy; this impact was quantified as the variance between observed and modelled results generated from a river impact model. The variance between EMC and ‘dynamic’ observed values to rainfall characteristics showed that these variances, whilst noticeable, may not be significant in contrast to observed variances when using ICM models made up of industry standard deterministic sewer and river water quality models. It was evaluated that there is significant potential for more widespread use of EMCs within integrated modelling approaches if a reliable EMC prediction methodology could be found.

The risks associated with the work presented in Chapter 3 are now discussed. The work used actual optimum EMC values derived from two observed water quality events, it must be noted that it is highly unlikely that an EMC water quality model would be able to consistently reproduce optimum EMC values; this likelihood is linked to the level of calibration of the complex model; the models ability to represent the sewer system accurately, in contrast, the complex models used in this study were calibrated to UPM and WaPUG regulatory criteria and were verified as suitable for use in ICM studies by the UK’S regulatory body; the EA.

Only one deterministic complex model was presented in this work, there are other available complex models with alternate pollutant description techniques, the use of these models may produce different results. It is there for a recommended that the work in chapter 3 be repeated using different complex models calibrated with the same water quality calibration data. In the context of the ICM model, further work regarding the simple description of pollutant events should be performed, this would give a broader appreciation of the differences and implications associated with using complex and simple dynamic pollutant description techniques. The study could also be performed using simple EMC methodologies already published within the literature to gain a more accurate understanding regarding the implications associated with both methods.

7.2 Evaluating the performance of EMC models using case study data

The objective of chapter 4 was to provide recommendations which could aid the development of a new water quality model. The use of previously developed EMC models to estimate pollutant concentrations has been achieved with mixed success, this success is inherently sensitive to the strength of available experimental data that can be used for calibration. It is generally agreed within the literature that TSS concentrations are the most important indicator of stormwater pollutant, thus the scope of the study was narrowed to the development of a new TSS EMC stormwater model.

Following presentation of a literature review concerning storm water processes and EMC models which try to describe these processes, it was established that land use characteristics, climatic and rainfall characteristics have an important impact on resulting TSS EMC pollutant concentrations but that establishing any explicit relationships which allow transferability of default model parameter values across catchments had previously been achieved with little success.

A new comprehensive water quality data set was presented in chapter 4, this data set was used to test a previously published EMC methodology presented within the literature to evaluate the transferability of this ‘simple’ approach to water quality modelling and establish the transferability of this approach. The study shows that a previously published empirical TSS model can be used to predict TSS event mean concentrations in catchments other than where it was first derived. The chapter concluded with the recommendation that simplified water quality techniques should include some explanatory variables which account for build-up and wash off processes.

Only one previously published TSS EMC model was tested in this study, whilst the number of TSS EMC models presented within the literature is limited, it is recommended that other simple pollutant techniques be utilised in the study set to gain further understanding as to the transferability of these simplified model’s.

Chapter 4 suggests that EMC’s are an adequate measure to assess pollution impact on a water course. The most important piece of legislation in this area is the Water Framework Directive (WFD) which aims to ensure all the EU’s surface water bodies are improved to a ‘good’ ecological status. Currently, different approaches are used in the UK; described in Chapter 2 Section 2.5. These approaches do not use EMCs but concentration-duration-thresholds (CDT)’s, this would suggest that the EMC approach may not be compatible with the WFD approach. The WFD is primarily concerned with achieving an outcome, namely, ‘Good’ status for all water bodies and describing what ‘Good’ status is e.g. for priority substances, there are concentration values that must not be exceeded (expressed as mean or maximum values). In general, the WFD is not very prescriptive about how the status objective is achieved, thus the extent to which the EMC approach proposed is compatible with the WFD is dependent on the extent to which it contributes to achieving ‘Good’ status? In essence; Is the EMC approach inferior to the CDT approach? In this regard, it can be argued that there are advantages and disadvantages associated with both the EMC and CDT approach. For example, although the CDT approach is more deterministic than the EMC approach, this doesn’t necessarily mean it is better since there are significant uncertainties on the extent to which the CDT approach might approximate reality. The EMC approach offers a less granular perspective but reduces the need to make assumptions that might be very difficult (or even impossible) to verify and test. The strength of the CDT approach is that it has been more strongly linked to observations of fish and invertebrate mortality, thus it can be argued to be more closely related to ecological status than EMC values. Importantly, this work is not focussed on replacing deterministic modelling with a simple modelling, the benefits associated with the EMC approach are that it can be used more readily as part of solution design testing analyses, thus It is concluded that if the EMC method doesn't fully comply with WFD requirements, the method can still be used to add to the pool of knowledge regarding the application of the ICM approach.

7.3 Development of a new stochastic TSS EMC model

This objective of chapter 5 was to develop a new model capable of predicting storm water TSS EMC’s, the structure of which incorporated build-up and wash-off components by utilizing explanatory variables which best described variations in TSS EMC’s.

A multivariate analysis technique was used on the new water quality data set presented in chapter 4 to explore build-up and wash-off explanatory variables that ‘best’ described the variations in TSS EMC’s. Mathematical derivation of the commonly used exponential decay function, often used to describe the behavior of catchment TSS storm water pollutants was carried out to develop a new TSS EMC model. After model development, a specific calibration algorithm was developed to explore different mathematical functions which ‘best’ describe the build-up and wash-off functions within the model. Following derivation of the optimal model structure and optimized parameter values, to gain understanding of model inputs and model parameters, a GSA analysis was performed using hypothetical input variables experienced during the study, the analyses revealed the importance of focusing water quality calibration campaigns on specified input variables and the extent to which parameters within the model impact model output results. An approach to evaluating the uncertainty was presented based upon model prediction and observed errors which could be used in conjunction with the model to quantity the uncertainty associated with model prediction.

In accordance with the literature, following visual analysis of the multi-variate analysis results, it was determined that the variable rainfall intensity (AGI5) described the largest variation in TSS EMC’s, furthermore, as the ADWP (antecedent dry weather period) was the only climatic variable available for analysis in the study, ADWP and AGI5 were selected for use in the development of a new TSS EMC model. Manipulation of the exponential wash-off equation was presented to develop a model structure capable of generating TSS EMC’s. Following application of the calibration algorithm to six different catchment data sets, results suggested that one of the seven different model forms described variations in TSS EMC’s significantly better than all other model formulations examined. In comparison to model efficiencies presented within the literature, the model had relatively ‘good’ predictive power in three of the six catchments to which is was applied (ER, RCW and SHEP), model performance on the remaining three catchments was considered ‘satisfactory’; showing significantly more predictive power than when using a mean of the observed water quality values recorded in these catchments. The relatively poor performance of the model in one catchment was attributed to the possibility of cross connections between surface and sewerage system. It of note, that limited information regarding the application of similar models is available within the literature, therefore any comparative evaluation regarding model performance is limited. Optimal model parameter values were relatively stable across all catchments, furthermore, model sensitivity analysis indicated that the model is sensitive to model parameter value C (associated with the wash-off component of the model), the model showed little sensitivity to parameter values b and d, suggesting that these could be fixed, however, it was concluded that as the GSA model inputs and parameter distributions were obtained through analysis of the water quality monitoring campaign and model development respectively, these distributions may not fully reveal the true sensitivity of the model, it is therefore recommended that alternate model and input distributions be used in future GSA studies associated with the model.

Analysis of model residuals (observed TSS EMC's versus model predicted TSS EMC's) suggested that the model tended to under predict catchment TSS EMC's, the resulting probability density functions for each catchment associated with the ratios of each catchments residual errors were found to be log normally distributed, whilst this could indicate a problem with the model structure, this was not investigated further, however, it has been stated in the literature that modelling error residuals could be log-normally distributed. A new TSS EMC model was successfully developed in chapter 5, the accuracy of the model outputs (related to its prediction performance) was relatively good in comparison to other studies, thus it was concluded that the objectives of chapter 5 were achieved.

The model development phase of chapter 5 could be improved by investigation into other possible climatic variables which could be used within the build-up component of the model. The land use characteristics in this study were broadly defined and ultimately showed no relationship with resultant TSS EMC's. A significant weakness in the model is the lack of accountability for accumulated loads on the catchment surface, this could have been a major source of residual error, however, the fact the model operates at the temporal event scale, is what provides inherent benefits associated with simple models of this kind, thus if an explanatory variable could be incorporated which reflected the amount of TSS remaining on the catchment surface following the event preliminary to the one under analysis, model performance could be improved.

7.4 Model transferability

The objective of chapter 6 was to study the implications associated with the application of the new model to catchments other than where it was initially developed, such that its application to new catchments in a practical context could be evaluated.

Due to a lack of water quality data available for model calibration in the UK catchments, a verified complex deterministic model was utilised to generate a synthetic water quality data with which the newly developed model could be calibrated and validated against. The model was then validated using data from the two-monitored water quality presented in chapter 3.

The model was applied to a catchment where water quality was available for only two water quality events, thus limited conclusions can be drawn as to the predictive capabilities of the model. However, the resultant TSS ECM's calculated from observed data were shown to fall between the upper and lower 95% confidence intervals through application of the Factor Ratio uncertainty technique developed in chapter 5. The high model efficiency values obtained for calibration and validation of the model to the synthetic water quality data set show that the model can successfully 'mimic' the complex description of water quality, furthermore, it does this at significantly reduced computation cost.

The work in chapter 6 could be improved by validating the model to more observed water quality events, offering further information regarding its transferability and predictive capabilities. The model is also dependent on hydraulic information provided by a complex model, due to its representation of TSS as EMC's, thus it could never be used as a standalone package.

The model was derived to predict stormwater TSS EMC's, this limits its application to combined sewer network catchments, whereby an inclusion of the wastewater component present and the impacts of in-sewer processes need be accounted for. It could be arguing that the models 'under' prediction of the two observed events on the Denton catchment which is combined could show that these if wastewater inputs and in-sewer processes were added to the model, application to combined systems could be achieved. Conversely, wastewater inputs tend to be more predictable and less susceptible to random fluctuations thus the inclusion of a wastewater input component could be achieved, however, incorporating a model component which accounts for how in-sewer processes affect final water quality predictions would be difficult as these in-sewer processes and interactions are not yet fully understood. It is there recommended that investigation into the model's application to a combined sewer water quality data and incorporation of model structure components representing wastewater generation and in-sewer model processes need be further explored, further implication of this would be that modelling complexity begin to increase.

Whilst the literature suggests that TSS is the most important indicator or urban pollution, the applicability of the model in a practical environment could be improved if the model had the capability to predict BOD, COD and NH_4 EMC's. Whilst it is hypothesized that some empirical relationship could be developed between TSS, BOD and COD, at present, the model is unlikely to be able to predict NH_4 due its association with inherent association with wastewater.

The model was developed on a water quality data set collected in Melbourne Australia, whilst the rainfall characteristics in Melbourne are similar to those experienced in the UK, collection of a comprehensive UK water quality data set similar to the monitoring campaign presented in chapter 4 would certainly offer more information as to the applicability of the model to new catchments.

Following calibration to the UK catchment, further work could be done which would significantly benefit chapter 3, whereby the potential of EMC pollutant description techniques could be evaluated using the newly developed model as oppose to the optimum EMC values recorded at each CSO, this would offer further information as to the potential of these EMC based techniques in the integrated context.

With many utilities currently in possession of verified complex sewerage network models, the potential for simple model to 'mimic' their complex description techniques could offer cost efficiencies in the practical environment. Subject to the efforts required to calibrate the model, the ability to quantity the uncertainty associated with its prediction allows for interpretation of probabilistic results, this offers decision makers using ICM approaches the opportunity to test, plan and develop solutions to urban drainage problems with increased information regarding the probability of success, furthermore, the opportunity to value solutions on the probability of their success provides information which could be considered valuable to numerous different stakeholders involved in the ICM process.

7.5 Summary of conclusions

To conclude, the main findings of this thesis are:

- There is potential for EMC pollutant description techniques to be used in ICM studies.
- Storm water EMC models should account for build-up and wash-off processes of pollutants within a catchment, preferably using an explanatory variable with respect to rainfall to describe variations in TSS EMC pollutant concentrations.
- There is a potential for EMC models to mimic their deterministic complex water quality, with respect to computation costs and uncertainty quantification, this potential offers increased efficiencies and opens up the interpretation of probabilistic results which could be used to aid the development of solutions in the ICM process.

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