

Optimal Design of Wastewater Treatment Plants Subjected to Time-Varying Inputs

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by

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**Abstract**

The objective of this thesis is to develop a computational framework for the optimal design of wastewater treatment plants that takes into account dynamic variations in both flow rate and wastewater compositions. These variations can be very large over the course of a year (e.g. +/-100%) and it is therefore important to explicitly take them into account in the design rather than relying on averaged values. Our approach is to minimize an economic objective function using a heuristic optimization algorithm (particle swarm). Since we use the detailed industry standard activated sludge model no.3 (ASM3), this problem is computationally very challenging. However, the presented work shows that this method is a very effective one. We demonstrate a cost saving of 67% when our novel method is compared with existing methods based on averaged inputs.

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**Notations and Abbreviations**

|  |  |
| --- | --- |
| ADM | Anaerobic digestion model |
| *ASett* | Cross-section area of settler |
| ASM1 | Activated sludge model no.1 |
| ASM2 | Activated sludge model no.2 |
| ASM3 | Activated sludge model no.3 |
| ASM3\_2N | Activated sludge model no.3\_2N |
| A2O | Anaerobic-anoxic-oxic |
|  | Coefficient of inlet flow rate |
| BBOD5 | Weighting factor for BOD5 |
| BCOD | Weighting factor for COD |
| BNO | Weighting factor for NO |
| BSS | Weighting factor for SS |
| BTKN | Weighting factor for TKN |
| BOD | Biochemical oxygen demand |
| BSM | Benchmark simulation model |
|  | Coefficient of recycle flow rate |
|  | Reactor concentration of component |
|  | Influent concentration of component |
| COD | Chemical oxygen demand |
| COST | European co-operation in the field of science and technical research |
| CSTR | Continuous stirred tank reactor |
| EQ | Effluent quality index |
| *FUS* | Fraction of non-biodegradable soluble COD proved by BioWin influent module |
| *FUP* | Fraction of non-biodegradable particulate COD proved by BioWin influent module |
|  | Non-settleable fraction of the influent suspended solids concentration to the settler |
|  | Fraction of biomass leading to particulate products |
| GAMS | General algebraic modelling system |
| IAWQ | International association on water quality |
|  | Investment cost for aeration system |
|  | Investment cost for influent pumping station |
|  | Investment cost for settler |
|  | Investment cost for sludge recirculation |
|  | Investment cost for tank |
|  | Total investment cost |
|  | Index representing for each component in the matrix |
|  | Mass of nitrogen per mass of COD in biomass |
|  | Mass of nitrogen per mass of COD in products from biomass |
| *J* | Objective function |
|  | Flux of particulate solids due to the gravity settling above the feed layer |
|  | Flux of particulate solids due to the gravity settling under the feed layer |
|  | Index representing for each process in the matrix |
|  | Half-saturation coefficient of substrate |
|  | Half-saturation coefficient of oxygen |
|  | Oxygen transfer coefficient |
| MINLP | Mixed integer nonlinear programming |
| MLSS | Mixed liquor suspended solids |
|  | Nitrogen gas |
| NLP | Nonlinear programming |
| NPV | Net present value |
| Ntot | Total nitrogen |
|  | Operating cost for aeration |
|  | Operating cost for external carbon dosing |
|  | Operating cost for effluent quality |
|  | Operating cost for pumping |
|  | Operating cost for sludge disposal |
|  | Total operating cost |
| ODE | Ordinary differential equation |
| OUR | Oxygen uptake rate |
| PPT | Proximate parameter tunning |
|  | Volumetric flow rate |
|  | Volumetric flow rate in the sedimentation zone |
|  | Effluent volumetric flow rate |
|  | Recycle volumetric flow rate |
|  | Volumetric flow rate to the settler |
|  | Wastage volumetric flow rate |
|  | Hindered zone settling parameter |
|  | System reaction term |
|  | Flocculent zone settling parameter |
|  | Substrate concentration |
|  | Input substrate concentration |
|  | Substrate concentration in the first reactor |
|  | Root of function |
|  | Substrate concentration in the second reactor |
|  | Minimum point of functions |
|  | Alkalinity of the wastewater |
|  | Inert soluble organic material |
|  | Ammonium plus ammonia nitrogen |
|  | Nitrite nitrogen |
|  | Nitrate nitrogen |
|  | Dissolved oxygen |
|  | Readily biodegradable substrate |
| SBR | Sequencing batch reactor |
| SRT | Solid retention time |
| TKN | Total Kjendal nitrogen |
| TSS | Total suspended solids |
|  | Max specific growth rate |
|  | Volume |
|  | Stoichiometric coefficient for components in the matrix |
|  | Max Vesilind settling velocity |
|  | Max settling velocity |
|  | Liquid velocity above the feed layer |
|  | Settling velocity in the layer |
|  | Liquid velocity below the feed layer |
| WWTP | Wastewater treatment plant |
|  | Biomass concentration |
|  | Biomass concentration in the first reactor |
|  | Biomass concentration in the second reactor |
|  | Autotrophic biomass |
|  | Heterotrophic biomass |
|  | Inert particulate organic material |
|  | Suspended solids concentration in the layer |
|  | The difference between suspended solids concentration in the layer and the minimum attainable suspended solids concentration |
|  | Nitrite-oxidizing autotrophs |
|  | Ammonia-oxidizing autotrophs |
|  | Particulate organic material |
|  | Slowly biodegradable substrates |
|  | Mixed liquor suspended solids concentration entering the settler |
|  | Suspended solids |
|  | Organics stored by heterotrophs |
|  | Substrate utilization rate |
|  | Hydraulic retention time (HRT) |
|  | Operating cost update term |
|  | Rate expression |

1. **Introduction**

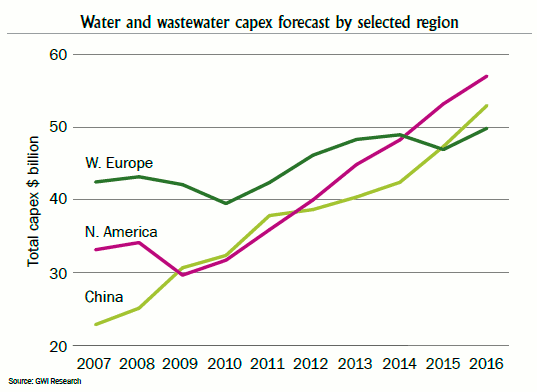
**1.1 Preface**

Every form of life is dependent on water and the daily water requirement for each species is significantly different. For example, the human body requires 2-3 liters of drinking water every day in order to maintain a healthy balance within the body([Jeppsson, 1](#_ENREF_37)996). Compared to other forms of life, mankind has the greatest influence on the quality of water as many of its modern activities involve the consumption of large quantities of water. This results in the accumulation of an immense volume of wastewater that, unless treated properly, potentially threatens public health and the environment due to the spread of water-borne diseases and toxic compounds.

The development of primitive wastewater management in developed countries can be traced to the early 1800s. Only a few wastewater treatment utilities were constructed for the collection of stormwater and drainage water. This resulted in a significant decrease in sanitary problems within cities, while hiding another issue, namely: the polluted wastewater. This, to a great extent, subsequently accelerated the development of more intensive wastewater treatment systems([Tchobanoglous and Burton, 1991](#_ENREF_52)). Due to the increase in the understanding of self-cleaning mechanisms in nature and in the requirement for a higher quality of discharged water, a number of treatment methods in the mid of 1900s were developed. The most commonly used approaches that biologically deal with wastewater are the activated sludge process and the anaerobic digestion process.

Wastewater treatment has become, by far, the largest industry in terms of volume or weight of treated raw materials ([Gray, 1989](#_ENREF_24)). Due to a rapid population expansion and booming industrial development, the increase in the discharge of huge amounts of wastewater from both domestic and industrial communities during the last few decades has become a critical problem. For example, in the UK, approximately 10 billion liters of sewage is produced daily and the energy required for plants to deal with this large volume of sewage is about 6.34 gigawatt hours per day, which is equivalent to 1% of the average daily electricity consumption of the UK (Parliamentary Office of Science and Technology, 2007)**.** Such high energy consumption along with the increasingly tighter water quality standards has significantly increased the operating cost of existing facilities as well as the investment cost for new wastewater treatment plants.

The expenditure trends for the future are illustrated in Figure 1.1. What is interesting about these predictions is that expenditure is expected to increase for both developed and developing countries alike. This data is based on a report (Global Water Intelligence, 2005) regarding the forecast of capital expenditure on wastewater treatment in three regions (North America, Western Europe and China) during the period of 2007-2016. In 2007, the investment in North America, Western Europe and China was significant, estimated as $42 billion, $33 billion and $23 billion respectively. Although, there was a slight decrease in spending in the first two regions till 2010, the trends afterwards reversed and the predictions for 2016 are $50 billion and $57 billion respectively. China seems to be the biggest future water market as the government shifts more emphasis towards environmental protection. Chinese expenditure is anticipated to rise annually from $23 billion in 2007 to $53 billion in 2016, exceeding that of the Western Europe by $3 billion.



**Figure 1.1** Water and wastewater capital expenditure forecast by selected regions (Global Water Intelligence, 2005)

There has been a gradual rise in water budgets every year all over the world to satisfy the demand for large quantities of purified water by the growing population. Despite this, some studies have revealed that even well-operated wastewater treatment plants are failing to meet the discharge effluent quality standards up to 9% of the time (Jeppsson, 1996). An example of surprisingly poor performance regarding the instability of existing treatment plants was recently reported by the Environmental Protection Agency (2012):almost 50% of wastewater treatment plants serving urban centers in Ireland failed to achieve national and EU standards. Such an issue is very common and pervasive for many wastewater treatment applications across the developed world. This poor performance determined can be attributed to many factors including: inflexible designs, overloading and inadequately trained operators as well as a lack of process control. To address these, there has been a fair amount of research dedicated to the use of modelling approach to improve plant design, performance and control. These include algorithmic approaches to solve process synthesis problems in order to identify one or more design alternatives that best meet the idealized plant target. These examples include: the development of discontinuous derivative nonlinear programming model (DNLP) for optimal synthesis and design for wastewater treatment plants (WWTPs) ([Alasino et al., 2007](#_ENREF_2)); the use of stochastic optimization techniques to search for a set of optimal design candidates for activated sludge plants to achieve robust performance targets based on a superstructure network ([Rigopoulos and Linke, 2002](#_ENREF_47)); the systematic development of mixed-integer nonlinear programming model for the optimal synthesis of the advanced oxidation process networks to minimize total wastewater treatment plant costs (Pontes and Pinto, 2011) and so on. All of this effort, however, only focused on optimization based on static models and the optimal designs achieved are considered as the optimal choice at a single point of time (i.e. for steady state operation). The systematic optimization of dynamic wastewater treatment models has not been reported in the literature. The development of a mathematical framework for the optimal design of wastewater treatment plants that simultaneously takes into account the dynamic variations in both inlet flow rate and wastewater compositions will be presented in this work. A subsequent comparison of the plant design using our dynamic approach to that obtained using averaged steady state data will be also discussed.

**1.2 Motivation**

The main drive to carry out the investigation on the optimal design of dynamic wastewater treatment processes can be divided into two major aspects, as follows:

* Health and environmental motivation:

The increased public awareness on health protection and environmental concerns over the last few decades has been reflected in closer monitoring of water quality. Due to the increased interest in contaminants in wastewater, as well as the concern of the spread of water-borne diseases, more stringent effluent regulations have been introduced. This has triggered the development of more sophisticated treatment approaches which aim to perform better on pollution removal (e.g. organic carbon and nitrogen).

* Economic motivation:

As a result of dealing with a large amount of wastewater discharged from both domestic and industrial applications over the past 20 years, many new wastewater treatment plants based on prior design knowledge or even a trial-and-error philosophy have been constructed. Unfortunately, due to the lack of applicable design methodology, many facilities are over-designed leading to unnecessarily large energy requirements and capital costs for pollution removal. Therefore, the need to develop a general method capable of optimizing designs in order to yield most cost-effective wastewater treatment plants is a high industrial priority.

**1.3 Objectives and Contributions of This Work**

The aim of this work is to improve the design and performance of biological wastewater treatment processes using computational modelling and mathematical optimization. Based on structured plant models, an objective function that represents the total plant cost required to treat variable inputs of wastewater to achieve a specific performance is thus formulated. This economic optimization problem is minimized by using a variety of optimization algorithms in order to yield a near optimal design flowsheet.

The major objective of the detailed work that we present on modelling of activated sludge process plants is to use the mathematical methods to represent the knowledge of the process dynamics, thus achieving the simplest models capable of explaining the biological degradation in the processes. Therefore, a simple motivating model dealing with the biomass () growth only dependent on the expense of a single substrate () in continuous reactors is initially investigated. This is to represent an example of the dynamic description of the basic biochemical process in the wastewater treatment as well as validating our research methodology that can be further implemented on more complex models. Another goal in modelling of the activated sludge process plant is to provide an accurate prediction of the plant performance. To this end, we also present a simulation of an industrial wastewater treatment plant subject to time-varying inputs that were captured over 25 days. This simulation approach for existing assets can assist the adjustment of operating parameters in order to given better process performance.

In this project, we have, for the first time, developed a computational framework for the optimal design of wastewater treatment plants that simultaneously takes into account dynamic variations in both feed compositions and flow rate. The major contributions of this work are summarized below:

* **Modelling: Adapting freely available system biology software for formulating and solving process synthesis problems**. Functionality, reliability, efficiency, user-friendliness and compatibility are the major factors to be considered when choosing appropriate software packages for modelling purposes. The models presented in this work are coded in system biology markup language (SBML) which is a common data format used in the majority of system biology packages. These models, therefore, can be freely shared with the research community and analyzed by others without any adaption. Four typical software tools having different user-interfaces to define models (e.g. through a textual form or a dialog box or an explicit network diagram) were used in this work. A key contribution of this work, therefore, is to provide a framework for process modelling and optimization that relies exclusively on freely available software.
* **Optimization: Comparison of a range of stochastic algorithms on a minimal wastewater process synthesis superstructure.** Choosing the most efficient and best performing algorithms for the challenging nonlinear programming problems in this work was of prime importance. Our validation involved a simple motivating example which was published and, importantly, amenable to analytical solution for the optimal plant configuration. This allowed the performance of a variety of numerical algorithms on the same problems to be assessed. In terms of accuracy of solution and the expense of computation, the particle swarm optimization, generating the minimum sum of squared error of residues in the simple model optimization, was selected as the dominating one to solve problems in the following work.
* **Application: Optimal design and manual retrofit of an industrial scale wastewater treatment process subjected to real time-varying influent data.**

Our dynamic formulation of this industrial problem had a time horizon of 9 months and a time granularity of 1 day. This resulted in an optimization problem that is two orders of magnitude larger than those solved previously and hence beyond the scope of deterministic mathematical programming approaches. By applying our combined modelling and particle swarm optimization methodology we are able to provide a modestly favourable comparison between our dynamic design approach and the averaged steady state approach. A separate strand of this work is the use of a specialized commercial wastewater simulation package (BioWin) to model the industrial plant with the same input data. Although this software lacks the ability to optimize process synthesis problem, it has detailed inbuilt models for biological wastewater treatment including clarification and anaerobic digestion. As an alternative approach to automation optimization, we propose a physical process retrofit by adding an energy recovery system onto the existing plant configuration. The allocation of appropriate sized anaerobic digestion model significantly saved the power consumed due to the aeration as well as minimizing the sludge production rate.

**1.4 Thesis Overview**

Chapter 2 presents a review of the literature and a general introduction to the two most widely used biological wastewater treatment methods: the activated sludge process and anaerobic digestion. It also provides a detailed description of Benchmark Simulation Model No.1 (BSM1), which provides a standardized procedure for model simulation and evaluation. The integrated process synthesis methodology is also discussed, which show its ability to search for optimal designs for industrial plants.

Chapter 3 describes the method employed in this research. The first part focuses on modelling of wastewater treatment plants by using mathematical techniques. This task is a five-step procedure, namely: synthesis of unit connectivity, process model design, model development in different simulator environments, mapping a system biology tool to process synthesis problems and validation. The second part describes the strategy of how to use the heuristic optimization algorithms to solve the design problems of industrial wastewater treatment plants.

Chapter 4 addresses the optimization of the simple motivating model by using a variety of optimization methods (e.g. analytical and numerical approaches). In spite of only considering two state variables (substrate and biomass), the model demonstrates key concepts and method validation for the dynamic description of the processes involved in more complex models.

Chapter 5 presents a case study of modelling an industrial wastewater treatment plant in China using a commercial software tool. Due to the lack of an optimization module in this tool, we decide to retrofit the existing configuration by adding anaerobic digestion models to yield renewable energy. This effect is to offset the energy consumed during the aerobic degradation stage.

Chapter 6, for the first time, explores the possible benefit of systematic optimization of the activated sludge process subject to time-varying inputs. Having proved the validity of the process model under steady state conditions, the model with time-varying inputs is simulated and optimized. A comparison between the optimal designs under two scenarios (the steady state and the dynamic state models) is subsequently carried out.

Chapter 7 provides a general conclusion for what we have done and suggests areas for future work to address the limitations and also extend the framework presented here.

1. **Literature Review**

**2.1 Preface**

In this chapter, we initially present an introduction to the field of biological wastewater treatment processes including the activated sludge process and the anaerobic digestion process. Using mathematical modelling, we can achieve an accurate prediction of the dynamic behaviour of these biological processes in wastewater treatment plants. The detailed models- International Water Association models ([Henze et al., 2000](#_ENREF_33)) that describe the biological reactions taking place in the activated sludge process are discussed in section 2.3. A review of the Benchmark Simulation Model developed by IWA Task Group on Respirometry-Based Control of the Activated Sludge Process (Copp, 2002) discussed in section 2.4 demonstrates a standardized model simulation procedure and a mathematical measure for evaluating plant performance. However, to determine a cost effective design for treatment plants using mathematical modelling in a trial-and-error fashion is time-consuming. Optimization can help identify one or more design alternatives that best meet the desired objective through an automated search among all design possibilities. A general introduction of optimization is given in section 2.5. We also introduce process synthesis methods used in chemical engineering applications in section 2.6.

**2.2 Wastewater Treatment (WWT)**

The original development of wastewater treatment methods was to respond to the concern for the public health and the adverse conditions caused by the discharge of wastewater to environment (Metcalf and Eddy, 2003). During that period, the treatment intentions focused primarily on the removal of solids and grit, then on the degradation of organic matter followed by the elimination of the pathogenic organisms. With an increased public awareness on aesthetic and environmental aspects, from 1960 to 1980, the earlier objectives were updated. This required an even higher reduction rate in Biological Oxygen Demand (BOD), suspended solids and pathogenic organisms as well as adding nutrient removal (nitrogen and phosphorous) for some specific cases ([Tchobanoglous and Burton, 1991](#_ENREF_52); Williams, 2005). The specification of higher levels of purification of treated wastewater can be attributed to: 1. an increased understanding of the environmental effect caused by wastewater discharges; 2. a full-scale improvement in the operation of unit processes in response to the discharge of some specific constituents in wastewater; 3. the rational utilization of water resources by the public and 4.the effective enforcement of specific quality indexes for treated wastewater by new guidelines and regulations (e.g. the Freshwater Fish Directive 78/649/EEC referring to the European countries). Since then, the treatment emphasis has been shifted to elimination of toxic and potentially toxic chemicals that may cause long-term health effects, while the early treatment objectives have continued. This resulted in the development of a number of different treatment and disposal approaches providing even better performances on pollution removal.

Nearly all modern wastewater treatment methods, depending on specific requirements, can be classified into the following types: physical, chemical and biological. In some cases, these unit operations and processes appear in a variety of combinations in treatment plants and the contaminants in wastewater are removed by the sequential steps which are summarized in Table 2.1.

**Table 2.1** Unit treatment processes

|  |  |
| --- | --- |
| Unit treatment process | Description |
| Preliminary treatment | Involves the removal of gross solids and grit. Such constituents, to a great extent, can cause maintenance and operational problems. |
| Primary treatment | Achieves the removal of suspended solid and organic matter from wastewater based on using physical operations such as screening and sedimentation. Effluent leaving this process contains a great amount of organic matter. |
| Secondary (biological) treatment | Involves the removal of biodegradable organics and suspended solids. With an increased public awareness on environmental protection, biological nutrients removal including nitrogen and phosphorous is also taken into consideration as a major treatment objective. |
| Tertiary treatment | The further step following the biological treatment process, which aims to eliminate BOD5, bacteria, suspended solids, specific toxic compounds in order to produce clean effluents that comply with the stringent discharge standards. The most frequently used unit processes include filtration and activated carbon. |
| Sludge treatment | As a result of biological metabolisms in reactors in wastewater treatment, sludge, together with organic matters in a form of flocculent, is generated. This processes that deal with the sludge removal are divided into the following sequential steps: the dewatering, stabilization, heat drying, thermal reduction and the ultimate sludge disposal. |

(Eckenfelder, 1998; [Gray, 1989](#_ENREF_24))

Because of focusing on the use of biological treatment methods (e.g. the activated sludge process and the anaerobic digestion process) to degrade organic carbon and nitrogen in water and wastewater, the knowledge of chemical and physical treatment methods will not be discussed in this work.

**2.2.1 The Activated Sludge Process**

Treatment methods that rely on biological activity to remove contaminants from wastewater are known as biological unit processes. Biological treatment is the most widely used process today, treating both industrial and municipal wastewater. In addition, the activated sludge process, among a variety of biological treatment methods, is the most effective one for the removal of carbonaceous and nitrogenous matter remaining in sewage. This process, in general, is based on the use of a variety of micro-organisms under aerobic conditions to oxidize dissolved and particulate carbonaceous organic matter and synthesis new biomass. As an essential nutrient to biomass growth, nitrogenous material in the wastewater is also consumed.

Aeration and sludge settlement are the two essential stages in the activated sludge process (Figure 2.1), in which five main components are involved and the details of which are summarized in Table 2.2. In the first stage, wastewater, after being processed from the primary sedimentation for the elimination of grit and gross solids, is introduced into the biological reactor where the mixed microbial population is maintained in suspension. The importance of the aeration environment in the reactor is that sufficient amounts of oxygen are provided to aerobes to sustain the relevant bioactivities, thus maintaining the flocs in a continuous state of agitated suspension. The approach to create such an environment is either by surface agitation or via submerged diffusers using compressed air ([Gray, 1989](#_ENREF_24)). Another process in the first phase is continuous mixing which aims to increase the oxygen mass transfer rate by achieving a maximum oxygen concentration gradient as well as ensuring adequate food to the biomass. The role of the sedimentation tank in the process is to guarantee an effective separation of the activated sludge from the treated effluent in order to meet discharge standards. The settled sludge is further recycled back to the biological reactors to maintain sufficient biomass remaining in the reactor for an adequate rate of organic matter removal.

Aeration basin

Returned activated sludge

Air

CO2

Effluent

Waste sludge

Wastewater

Sedimentation

tank

**Figure 2.1** Flowsheet diagram of the activated sludge process (Vesilind, 2003)

**Table 2.2** Process components of the activated sludge process

|  |  |
| --- | --- |
| Process component | Functionality |
| Reactor | In tanks or ditches, adequate mixing between incoming wastewater with micro-organisms and aeration can be ensured. |
| Activated sludge | It is a flocculent suspension of all types of bacteria cultivated in tanks. Named as mixed liquor suspended solids, its optimal concentration is usually in a range of 5000-6000 mg l-1. |
| Aeration system | Dissolved oxygen in reactors for metabolic activities is either supplied through surface aeration or diffused air. |
| Sedimentation tank | The placement of a settlement tank at the end of the activated sludge process is to separate the activated sludge from the treated effluent. |
| Recycled sludge | After being separated from the sedimentation tank, the activated sludge is recycled back to the aerobic reactor in order to maintain sufficient biomass for pollution degradation. |

(Bitton, 1994)

**2.2.1.1 Evolution of the Activated Sludge Process**

The early use of wastewater purification can be traced back to the late 19th century when a means of supplemental aeration based on the fill-and-draw approach popularized. Wastewater was initially filled into reactors, further aerated and released. The remaining solid was then removed as waste. A subsequent development by Ardern and Lockett (1914) based on the existing process in 1914 resulted in the activated sludge process. After repeating the aeration on solids in wastewater, an increase in purification capacity and a decrease in substrate concentration were simultaneously found. In addition, the substrate removal rate was also dependent on the proportion of flocculent solids retained in the system. The same conclusion was afterwards determined by many other researchers all over the world (such as Bartow and Mohlman (1916) achieved this finding in the purification of swage by aeration in the presence of activated sludge, Clark and Adams (1914) published the same outcome through ‘sewage treatment by aeration and contact in tanks containing layers of slate’ and so on). Some efforts in 1917 successfully adapted the principle to be operated under continuous-flow conditions in wastewater treatment. This involved the introduction of a diffused air process, leading to the construction of many new large-scale plants (Buswell, 1923). However, due to a rapid increase in water usage either by domestic or industrial applications every year, significant variations in flow rate and organic carbon load caused several operating problems. For example, the imbalanced food and a high carbon-nitrogen ratio supplied in the influent due to industrial discharges in aerobic reactors may favour the growth of filamentous bacteria, thus weakening the degradation of COD by the activated sludge and further resulting in a high concentration of suspended solids in the effluent. Another common issue to be considered was the insufficient supply of oxygen to the aeration tanks, which limits the growth of aerobes.

To avoid the aforementioned difficulties as well as achieving high effluent qualities, a great amount of effort was devoted to the improvement of the activated sludge process performance in terms of COD removal and these results were reported by Grant et al in 1930. For example, the multiple-points dosing activated sludge process introduces the feeding of regulated amounts of sewage to the system in order to ease the high demand for oxygen from the activated sludge due to the effect of shock loads, thus generating an activated sludge with a good purifying capacity as well as maintaining a stable dissolved oxygen level throughout the reactors (Gould, 1942). The introduction of this ‘tapered’ aeration also deals with the problem of a frequent shortage of oxygen in the aerobic units. An increase in the number of diffusers at the head of the aeration tank and a decrease in the amount at the outlet elevate the concentration of dissolved oxygen and its transfer rate in the reactors. This method is also used in some existing treatment plants (Kessler and Nichols, 1935). An attempt to develop high capacity aeration devices was also reported (Setter et al., 1945). Such a modification reduces the conventional aeration period with adequate oxygen supplied to systems, while allowing an increase in the sewage loads by reducing the floc size under a high degree of turbulence. The shortened hydraulic retention time and the increased substrate to biomass ratio also ensure the micro-organisms maintain a very active phase. The process thus is found to be more prevalent in small scale plants. Being competitive with the conventional techniques, sequencing batch reactor (SBR) operating based on the fill-and-draw basis for nutrient removal has been widely used since 1980s (Okada and Sudo, 1985; Manning and Irvine, 1985). In spite of utilizing a single tank, the biological conversion and settling can be sequentially carried out. As processes are governed by time rather than by space, it is found to be very flexible to handle variable operating conditions. The common unit processes involved are divided into five sequential steps: 1. fill, 2. react, 3. settle, 4. draw and 5. idle. First, the fill of substrate to the biological reactor may last for 25 percent of the full cycle time, which ensures a minimum of 25 percent of liquid level of the unit capacity. The biological reactions, lasting for 35 percent of the total cycle time, take place simultaneously during the fill. The aim of settlement is to separate the sludge from the clean effluent, which occurs when the aeration and mixing are switched off. In terms of purification capacity, SBR is highly effective as the contents in the settling mode are completely static. The time period for the removal of clarified treated water is in a range of 5 to 30 percent of the full cycle time and the idle process that allows the transition to another cycle in most cases is ignored (Dennis and Irvine, 1979).

By either increasing the oxygen transfer rate or adjusting the feeding strategy, these modified processes, to a great extent, were found to be quite effective for the degradation of carbonaceous material in wastewater. However, nutrients (nitrogen and phosphorus) removal due to the introduction of stricter regulations on effluent quality has become a major problem in wastewater treatment. One that combines aerobic, anoxic and anaerobic conditions into a compact activated sludge configuration allows different micro-organism species to function effectively for the removal of organic carbon and nutrients through a two-step of nitrification and denitrification process (Jeppsson, 1996). In general, organic nitrogen in wastewater is present in the form of proteins and urea. After being hydrolyzed, the ammonia-nitrogen can be either eliminated from wastewater by biological activates of micro-organisms through assimilation which incorporates nitrogen into cell mass or through nitrification-denitrification where nitrogen, in the first step, in the presence of oxygen, is converted into other nitrogen-form products. These are nitrite (an intermediate oxidized nitrogen product) and nitrate which, further can be converted into an ultimate gaseous product () through denitrification. Serving as an electron donor, the carbonaceous organic substance provides the essential energy source for denitrification. It is commonly expected to maintain the consumption rate at a maximum level in order to achieve sufficient nitrogen removal and to minimize the aeration cost.

Given that the aim of the research presented in this thesis is to use mathematical methods to generate optimal configurations for biological treatment plants, it is instructive to consider the evolution of process configurations that have been manually developed over the years based on sensible biological and engineering considerations. The configurations are mainly aimed at optimizing the dual wastewater treatment objectives of carbonaceous material removal (requiring aerobic conditions) and nitrogen removal (requiring anoxic, or very low oxygen levels). The energy source that is utilized by facultative bacteria in nitrification-denitrification systems can be either internal or self-generated (Van Haandel et al., 1981). The first process configuration utilizing an internal energy source in the influent for denitrification was proposed by Ludzack & Ettinger(Figure 2.2a) in 1962. A partial communication between an anoxic and an aerobic reactor is suggested and the influent is directly fed to the anoxic reactor. Due to the absence of oxidized nitrogen in the feed, it requires to recycle the oxidized nitrogen generated in the aerobic reactor to the anoxic reactor for denitrification. However, poor performance on the reduction of total nitrogen was obtained. A subsequent modified Ludzack & Ettingerconfiguration (MLE) (Figure 2.2b) separates the reactors into two individual units. In spite of achieving a better performance, the internal energy source-based processes cannot yield a nitrate-free effluent, indeed a significant portion of nitrate simultaneously leaves in the effluent.

(b) Modified Ludzack Ettinger

(c) Wuhrmann

(d) Bardenpho

(e) Modified activated sludge

(a) Ludzack Ettinger

Liquid

Sludge

Anoxic reactor

Aerobic reactor

**Figure 2.2**Single sludge nitrification-denitrification activate sludge process configurations, (a) Ludzack Ettinger (b) Modified Ludzack Ettinger (c) Wuhrmann (d) Bardenpho and (e) Modified activated sludge

(Van Haandel et al., 1981)

The self-generated energy source-based activated sludge systems rely on the energy extracted from the endogenous death and lysis of bacteria. The placement of an aerobic reactor at the front of the network is of necessity, as it provides aerobes a favourable environment in which to grow. The allocation of an anoxic zone following the aerobic reactor enables denitrification to take place at the expense of carbonaceous material from decayed bacteria. There is also a recycle stream that conveys the sludge from the anoxic unit to the aerobic unit in order to maintain sufficient biomass for oxidation of the organic carbon and nitrification. The configuration of this kind was firstly proposed by Wuhrmann (1964). However, because of low rate of energy release from organism death and lysis, it is hard to maintain a stable transformation process (nitrate to nitrogen gaseous) in the anoxic reactor. Many experiments, however, have been proved that nitrification efficiency may be affected as nitrifiers in the aerobic unit with a shortened hydraulic retention time will stop reproducing and hence ceasing the nitrification. Barnard (1973) proposed a combination of the MLE and Wuhrmann processes (Figure 2.2d). The repeat arrangement of anoxic-aerobic units yields two reaction zones where the pre-denitrification process (the 1st anoxic-aerobic) is followed by a post-denitrification (the 2nd anoxic unit). This configuration is to obtain low nitrate concentration in the effluent as well as stripping nitrogen gas bubbles from floc by adding a flash aeration reactor between the secondary anoxic reactor and the sedimentation tank. The enhanced biological phosphorous removal (EBPR) (Figure 2.2e)in the conventional activated sludge system was also proposed by Barnard (1976) when conducting a pilot-plant for nitrogen removal. By adding an anaerobic reactor in front of the pre-denitrification reactor to receive the recycled sludge, phosphorus in mixed liquor in the anaerobic reactor is thus released from the organism mass. Along with the feed from the influent, all the phosphorous in the following process is thus consumed by the bacteria.

Apart from these processes given in Figure 2.2, some other alternative configurations based on prior design knowledge or the trial-and-error pilot plants have been developed in the last 20 years in order to establish a trade-off between effluent quality and operating costs in the activated sludge process. Among these designs, systems under steady state and dynamic loadings have been tested and evaluated respectively and the most representative ones include the membrane bioreactor (Brindle & Stephenson, 1996), the alpha process (Ayesa et al., 1998), the batch as well as the sequencing batch arrangements(Zaiat et al., 2001) and the alternating plant (Zhao et al., 1995). However, a further description of these designs lies beyond the scope of this work.

**2.2.2 The Anaerobic Digestion Process**

Anaerobic processes are the other biological-based approach for treating sludge and high strength of organic wastes, especially animal waste and organic effluents from food processing industries (Gray, 1989). Among a variety of configurations that have evolved during the last ten years shown in Figure 2.3, the complete-mix anaerobic digestion is the most sophisticated one that has been widely used in many industrial applications. Organic material in mixed liquor suspended solids in this process, in the absence of oxygen, is biologically degraded and further converted into a number of end products including methane and carbon dioxide. Anaerobic digestion is commonly used to treat and destroy sludge from aerobic waste treatment, hence lowering sludge disposal costs. Compared to aerobic treatment methods, it has a number of advantages, such as less energy required (no aeration) as well as the possibility of energy recovery due to methane production. However, its widespread adoption for large scale wastewater treatment has been limited by significant disadvantages, such as: longer start-up times and solid retention times; the need for alkalinity addition; elevated temperatures (35 0C for mesophilic processes); and the frequent necessity of further treatment.

Gas

Gas

Feed

(b) Anaerobic contact process

Gas

Recycle

Feed

1. Completely mixed anaerobic

Digestion

Gas

Feed

Feed

(b) Upflow packed bed

(d) Downflow packed bed

Gas

Gas

Recycle

Feed

Feed

(e) Fluidized bed

(f) Expanded bed

**Figure** **2.3** Typical reactor configurations used in anaerobic wastewater treatment (Speece, 1983)

The biological conversion processes involved in anaerobic digestion can be divided into three steps (Figure 2.4): hydrolysis, fermentation and methanogenesis. The first step describes the enzymatic breakdown of complex organic molecules into simple soluble molecules which are treated as a source of energy and carbon for cell biomass. Substrates from the feed are initially decomposed into soluble compounds (protein, fat and carbohydrate) which are further hydrolyzed into basic structural building blocks including amino acids, long-chain fatty acids and monosaccharides. During the next stage, fermentation, the hydrolyzed compounds act as both electron donors and (in the absence of oxygen) as electron acceptors. They are broken down into acetate, hydrogen, carbon dioxide and propionate and butyrate through a variety of biochemical pathways. Methane formation in the final step is carried out by two types of micro-organisms respectively. Aceticlastic methanogens are responsible for the breakdown of acetate into methane and carbon dioxide. Hydrogen utilization methanogens utilize carbon dioxide as the electron acceptor and hydrogen to generate methane. The amount of methane produced through the conversion of acetic acid (the first route) can be limited due the low growth rate of bacteria (Benefield and Randall, 1980).

Stage 3

Methane formation

Stage 2

Acid formation

Fat acid

Ammonia acid

Monosaccharide

Complex particulate waste with active biomass

Fat

Protein

Carbohydrate

Stage 1

Hydrolysis

Monosaccharides

Fatty acids

H2O, CO2, formate, methanol etc

Methane and CO2

**Figure 2.4**The anaerobic digestion process

(Benefield and Randall, 1980)

As was previously mentioned, one of the greatest concerns for designers or practitioners working on wastewater treatment plants is in relation to energy recovery/energy saving during the operation. In the activated sludge process, the demand for sufficient dissolved oxygen for biomass growth is so high that strong aeration is required. This results in an energy intensive process and a large number of existing plants are now seeking to rectify this using retrofits. More specifically, by integrating an anaerobic digestion process model onto the aerobic activated sludge plant, a certain quantity of renewable gaseous methane can be generated. This, thus, can offset some energy used during the aeration and, additionally, can also improve performance. To accomplish such a process synthesis by means of computational modelling is the topic of chapter 5 which uses a detailed model simulation of an industrial case study.

In this study we demonstrate the use of biological treatment processes to achieve organic carbon and nitrogen removal in water and wastewater. We consider integrating mathematical modelling with the biological processes to reveal details of internal cause-effect relationship and further implement optimization algorithms to improve the performance of wastewater treatment plants. The detailed information of these two tasks is discussed in the following sections.

**2.3 Modelling**

Mathematical modelling is the key approach employed in this work to deal with the design of wastewater treatment plants. A general overview of modelling of systems, its advantages compared to manual methods and procedures for model construction are now discussed.

**2.3.1 The Importance of Modelling**

Model is defined as a representation or description of the properties of some objects or events in the real world (Stockburger, 1996). However, a model does not contain every aspect of reality. The basic principle to construct a model is that model should be accurate and concise as well as revealing details of internal cause-effect relationship within processes. Due to a rapid development of computer resources during the last few decades, a great many models throughout many disciplines have been explored. In spite of having a variety of types, such as linguistic models, visual models, physical models and mathematical models, we will restrict ourselves to the use of physical and mathematical (mechanistic) models. The former of these can, for example, indicate how the essential components can be connected, as in the type of process synthesis problem relevant to this work, with the network layout displayed as blocks connected with lines (Henze, 2008). Mathematical models are expressed as equations that relate inputs to outputs and are characteristic of the system under study.

A mathematical model is an excellent tool for conceptualizing the knowledge of a process so that people can understand, analyze and manipulate. A well-defined model can provide an accurate prediction of system behaviour for different conditions, thus allowing the further process optimization for specific purposes. This approach is treated as an alternative to laboratory experiments which inherently have a number of serious limitations. Mathematical models can deal with static systems (i.e. assumed to be at steady state) and dynamic systems. A number of advantages of using mathematical models to represent the activated sludge process are shown as follows:

* Getting insights into process performance
* Easy to upgrade/retrofit
* Diversifying the control schemes
* Saving time and money
* Minimizing the risks and understanding uncertainty

It is certain, therefore, that plenty of benefits can be obtained if an appropriate model for a wastewater treatment plant can be developed. However, the following points, which effect model accuracy, should also be considered:

* Adequate and accurate information regarding wastewater characterization and reactor hydraulics should be provided prior to model initialization.
* Sufficient variables and parameters should also be identified for model simulations and evaluation: e.g. multiple versions of each reaction and species for each process compartment in which they might occur.
* Meaningful published experimental or industrial data is required to validate the model results. (Orhon et al., 2009)

**2.3.2 Model Construction**

As alluded to earlier, mathematical modelling can provide an accurate prediction of the input-output behaviour of wastewater treatment plants and allow engineers and designers to achieve key objectives such as improved process performances. The essential steps to completely build such a model are summarized in Figure 2.5.

Verbal model

Mathematical model

Experiments

Verification

Use

**Figure 2.5**Model construction methodology

([Petersen et al., 2002](#_ENREF_45))

According to Figure 2.5, the first step is to setup the verbal model that contains the essential process elements including operating parameters, variables and process structure. The mathematical model, expressed in a form of ordinary differential equations in this research, describes interactions between each component in the process. The step of verification considers the validity of model responses. Models can only be used when their outcomes fit the data given in practical experiments or other published models. Failed validation may lead to iterative checks on the feasibility of the previous verbal model.

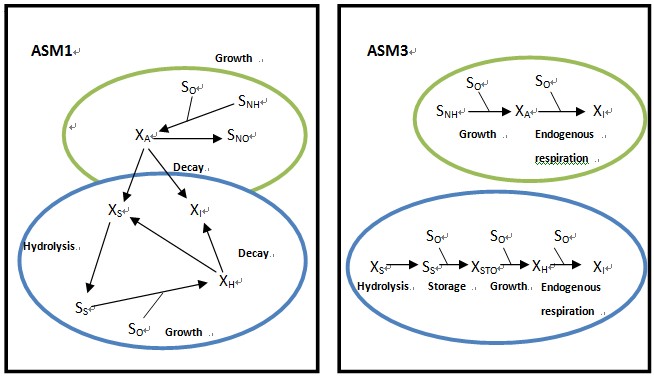
It should be noted that, in this work, the transition of the conceptual design into mathematical models that takes place during the model construction process is followed by process synthesis (section 2.6) in which the optimal plant configuration is sought. For a complete process synthesis methodology, a few prerequisites before the model construction should also be concerned, such as database formation and flowsheet preparation, the details of which can also be found in section 2.6.

**2.3.3 The Activated Sludge Model (ASM)**

To facilitate the development of wastewater treatment process models as well as its practicability, the International Association on Water Quality formed a task group in 1983. The group engaged in a research of the simplest mathematical models that have the capability of predicting the performance of the activated sludge process in terms of carbon oxidation, nitrification and denitrification ([Henze et al., 1987](#_ENREF_33)). As a result, Activated Sludge Model no.1 (ASM1) adapting several key concepts of the model by Dold et al (1980) was presented in 1987. ASM1 divided the major biological process into 8 sub-processes. According to the biodegradable characteristics of COD, the model further classified the organic carbon into biodegradable, non-biodegradable and biomass and the micro-organism can only grow at the expense of biodegradable fractions. This model was based on new experimental findings and was successively improved and extended, resulting into a number of evolved types, for example, ASM2 and ASM2d (Henze et al., 1995; Henze et al., 1999) mainly focuses on phosphorous removal and ASM3 (Gujer et al., 1999) deals with substrates stored within cells.

ASM3 (Figure 2.6a), adopted in this study, is widely used for representing biological transformation processes taking place in the activated sludge reactors. Although, similar to ASM1 (Figure 2.6b), it has corrected some of its defects. For example, based on the observations from the oxygen uptake rate tests (OUR) with the activated sludge unit, ASM3 introduces a new concept that readily biodegradable COD () is initially taken up by bacteria and further stored as an internal substrate () before being assimilated into biomass (Gujer et al., 1999). In ASM1, on the other hand, was defined as partly soluble and partly particulate, with no additional storage reaction. Another reason to introduce ASM3 is that the carbon cycle routine describing the transition of particulate COD from the decay process into readily COD for biomass growth has been removed from this model. This thus reduces the significant influence on the model results resulting from the minor change of a single parameter and achieves better accuracy for model calibration (Gernaey et al., 2004). The last and greatest innovation is to disintegrate the total oxygen consumption into three processes, namely: rapid oxygen consumption for RBCOD degradation; slower oxygen consumption for SBCOD degradation; and slower oxygen consumption for endogenous OUR. With the aid of these additions, the profile of the oxygen determined from the experimental practices can be better explained ([Henze, 2008](#_ENREF_32)).

Compounds in AMS3 are classified into soluble and particulate compositions which are denoted by and , respectively. Contributing to the formation of the activated sludge, the particulate compounds usually suspend in reactors by means of flocculation. Most soluble compounds provide the living cell food to grow. It is aimed to keep their concentration as low as possible in the effluent. The organic compounds in ASM3 are characterized by an index, chemical oxygen demand (COD) which divides carbon material into a number of fractions based on the nature of biodegradability. Figure 2.7 below displays the distribution of the COD components used in ASM1 and ASM3.



**Figure 2.6** (a)Flow of COD and nitrogen source in ASM1.**Figure 2.6** (b) Flow of COD and nitrogen source in ASM3 ([Henze et al., 2000](#_ENREF_33))

Total COD

Biodegradable

COD

Non-biodeg.

COD

Soluble

Particulate

Heterotrophs

Autotrophs

Soluble

Particulate

Active biomass

**Figure 2.7**COD decomposition tree

(Jeppsson, 1996)

Firstly, the total COD in ASM3 is divided into biodegradable COD, non-biodegradable COD and active biomass. The biodegradable COD is further split into readily biodegradable COD () and slowly biodegradable COD (). Consisting of simple molecules, the readily biodegradable COD in ASM3 is rapidly taken up by heterotrophic organisms and then stored in the cell as internal substrate () on which the growth occurs. While slowly biodegradable COD, comprising particulate/complex organic molecules, has to undergo hydrolysis before it is ready for degradation. The non-biodegradable COD including soluble inert () and particulate inert () material is treated as a fraction that is unaffected by any bioactivities. As a part of the influent composition, the soluble inert () is directly discharged from the effluent. Due to its insolubility, the particulate inert () accumulates with other particulates in the reaction compartments to flocculate with the activated sludge. The suspended solids (), which is not taken into account as a fraction of COD, is also introduced into the process kinetics to facilitate the prediction of mixed liquor suspended solids () as observed in the reactors. It is hypothesized that heterotrophs () and autotrophs () are the major classes of organisms to achieve COD and nitrogen removal. Heterotrophs, as facultative bacteria, are responsible for the hydrolysis and denitrification where nitrate is reduced to nitrogenous gas. Autotrophs, under aerobic conditions, are responsible for nitrogen removal through the nitrification reaction in which nitrogen is directly oxidized into nitrate. Other soluble compounds that are not included in Figure 2.7 also play indispensable roles. For example, dissolved oxygen () is essential for aerobes to conduct their reactions (nitrification and aerobic growth of heterotrophs). The pool of ammonium and ammonia nitrogen () is the major nitrogen source responsible for nitrifying organisms’ growth.

**2.3.3.1 Model Processes**

ASM3 represents the main biological transformation processes in the activated sludge process. The details of these processes are discussed by Henze et al., (2000) as follows:

* Hydrolysis: Hydrolysis in ASM3 (Figure 2.6 b) has less influence on the rate of oxygen consumption and denitrification than it has in ASM1. As the primary step, it makes all slowly biodegradable COD () in the influent available to biomass in the activated sludge process.
* Aerobic storage of readily biodegradable COD (): This introduces the concept that the readily biodegradable COD is firstly stored into the inside the cells in a form of storage products and is then absorbed to make biomass. Most energy required to achieve this is obtained from aerobic respiration. In spite of not being directly observed in real systems, this concept in the model can explain why the dissolved oxygen consumption rate is maintained at a very low level at the early stages when growth rates are still quite low.
* Anoxic storage of readily biodegradable COD (): This is similar to the aerobic storage process mentioned above, but the energy required in this process is obtained from denitrification rather than the aerobic respiration. The anoxic heterotrophic storage rate is assumed to be a relatively low value as a small quantity of heterotrophic biomass in the model is for denitrification.
* Aerobic growth of heterotrophs (): As the readily biodegradable COD has entirely been converted into the storage product , the heterotrophic biomass growth in this model will only take place at the expense of storage product .
* Anoxic growth of heterotrophs (): Similar to the aerobic growth, but denitrification takes place and nitrate is converted into nitrogen gas. A reduced anoxic storage rate compared to the aerobic case is observed.
* Aerobic endogenous respiration: This process considers all forms of biomass loss under aerobic conditions including decay, endogenous respiration, lysis, predation, motility, death and so on. Its mechanism is totally different from the decay process in ASM1.
* Anoxic endogenous respiration: Similar to the aerobic endogenous respiration, but a small portion of nitrate is expect to be denitrified into nitrogen gas.
* Aerobic respiration of storage product (): This process ensures the storage products decay with biomass.
* Anoxic respiration of storage product (): This process also describes storage decay, but under anoxic conditions.

**2.3.3.2 Process Kinetics**

To be mathematically tractable while providing realistic predictions, the IWA task group, based on the work of Petersen (1965), concluded a matrix format (Table 2.3) for representing the process kinetics of wastewater treatment models. All relevant biological processes with appropriate rate expressions (denoted by ) and the essential components in the model are characterized with indices and respectively. In addition, the stoichiometric coefficients that set out the mass relationship between these components in each individual process are denoted by . The system reaction term is the sum of the products of the stoichiometric coefficient and the process rate expression for component .

where: the index represents the different components, ranging from 1-13. The index represents each process and ranges from 1-9. is the reaction term for component .

The process rate expressions given in Table 2.4 are formulated based on Monod kinetics which represents a kind of switch function. The introduction of such a concept reflects the impact of required nutrients or inhibiting environmental conditions on biomass growth. Especially for the reactions that require electron acceptors, the switch function plays an indispensable role. For example, autotrophic biomass only reproduces in the presence of dissolved oxygen in reactors, so its corresponding switch function is defined as: . In this expression, is the concentration of oxygen and is the half saturation parameter- i.e. the value of oxygen concentration for which the expression attains a value of half. is often a very small value compared to the air saturated value, and the aeration should be sufficient to ensure that the oxygen concentration is several times this value to ensure that the expression is closed to unity- i.e. that oxygen is not a nutrient that is limiting to growth. Since the expression is used multiplicatively in the growth expression, it can be seen that growth (nitrification) will stop (become switched off) if the level of dissolved oxygen becomes zero. However, oxygen also acts as an inhibitor of the growth of anoxic organisms and this is modelled in the rate equation of such processes using the expression: in which dissolved oxygen acts as an inhibitor, limiting the growth of denitrifiers. The process of denitrification proceeds at its maximum rate when the dissolved oxygen converges to zero ([Peide et al., 2010](#_ENREF_44)) and, as the value ofincreases, the rate drops. In the context of inhibition, therefore, the parameter now controls the inverse relationship between growth and the oxygen inhibitor. If often has a very small value, indicating that denitrification is strongly affected by even low levels of oxygen and values that are several times above the value of will effectively switch this process off.

**Table 2.3** Process kinetics

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Compound | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 |
| process | *SO2* | *SI* | *SS* | *SNH4* | *SN2* | *SNOX* | *SALK* | *XI* | *XS* | *XH* | *XSTO* | *XA* | *XSS* |
| Expressed as | O2 | COD | COD | N | N | N | Mole | COD | COD | COD | COD | COD | SS |
| 1.Hydrolysis |  | 0 | 1 | 0.01 |  |  | 0.001 |  | -1 |  |  |  | 0.75 |
| Heterotrophs activity | | | | | | | | | | | | | |
| 2.Aerobic storage of Ss | -0.15 |  | -1 | 0.03 |  |  | 0.002 |  |  |  | 0.85 |  | 0.51 |
| 3.Anoxic storage of Ss |  |  | -1 | 0.03 | 0.07 | -0.07 | 0.007 |  |  |  | 0.8 |  | 0.48 |
| 4.Aerobic growth of XH | -0.6 |  |  | -0.07 |  |  | -0.005 |  |  | 1 | -1.6 |  | -0.06 |
| 5.Anoxic growth |  |  |  | -0.07 | 0.3 | -0.30 | 0.016 |  |  | 1 | -1.85 |  | -0.21 |
| 6.Aerobic endog. respiration | -0.8 |  |  | 0.066 |  |  | 0.005 | 0.2 |  | -1 |  |  | -0.75 |
| 7.Anoxic endog. respiration |  |  |  | 0.066 | 0.28 | -0.28 | 0.025 | 0.2 |  | -1 |  |  | -0.75 |
| 8.Aerobic respiration of XSTO | -1 |  |  |  |  |  |  |  |  |  | -1 |  | -0.6 |
| 9.Anoxic respiration of XSTO |  |  |  |  | 0.35 | -0.35 | 0.025 |  |  |  | -1 |  | -0.6 |
| Autotrophs activity | | | | | | | | | | | | | |
| 10.Aerobic growth of XA | -18.04 |  |  | -4.24 |  | 4.17 | -0.6 |  |  |  |  | 1 | 0.9 |
| 11.Aerobic endog. respiration | -0.8 |  |  | 0.066 |  |  | 0.005 | 0.2 |  |  |  | -1 | -0.75 |
| 12.Anoxic endog. respiration |  |  |  | 0.066 | 0.28 | -0.28 | 0.025 | 0.2 |  |  |  | -1 | -0.75 |

([Henze et al., 2000](#_ENREF_33))

**Table 2.4** ASM3 processes

|  |  |  |
| --- | --- | --- |
|  | Process | Process rate equation |
| 1 | Hydrolysis |  |
| Heterotrophic organisms, aerobic and denitrifying activity | | |
| 2 | Aerobic storage of Ss |  |
| 3 | Anoxic storage of Ss |  |
| 4 | Aerobic growth |  |
| 5 | Anoxic growth  (Denitrification) |  |
| 6 | Aerobic endogenous respiration |  |
| 7 | Anoxic endogenous  respiration |  |
| 8 | Aerobic respiration of  XSTO |  |
| 9 | Anoxic respiration of  XSTO |  |
| Autotrophic organisms, nitrifying activity | | |
| 10 | Aerobic growth of XA  (Nitrification) |  |
| 11 | Aerobic endogenous  respiration |  |
| 12 | Anoxic endogenous respiration |  |

([Henze et al., 2000](#_ENREF_33))

**2.4 Benchmark Simulation Model**

Due to the lack of a standardized procedure to efficiently assess the performance of numerous control strategies on activated sludge process plants, there existed a dispute among a variety of designs about which ones could bring better performance. To eliminate this doubt and to ensure unbiased comparisons among control strategies as well as providing a basis for model validation if experimental data is not available, the first benchmark (BSM no.1) was devised by the IAWQ task group on Respirometry-Based Control of the Activated Sludge Process(Alex et al., 1999). This benchmark was further modified by the European Co-operation in the field of Science and Technical Research (COST) together with the second IWA Respirometry Task Group (Copp, 2000; Alex et al., 1999; Pons et al., 1999). Limited to the evaluation of plant control strategies on short-time scale, an extension based on BSM no.1 to a long-time scale of plant-wide control has been proposed and named as BSM no.2, which additionally includes the pre-treatment process with a primary clarifier, the sludge treatment process, anaerobic digester and dewatering unit.

In fact, this benchmark model is mainly related to the evaluation of different control strategies and provides a basic simulation output in order to reflect the impact of control strategies on model responses. Advanced process control, however, is beyond the scope of this study. We rather focus on fact that the benchmark model is capable of providing a valuable set of output data for process design. This can be used as a basis for the verification of the behavior of the activated sludge process models using different process configurations.

The benchmark simulation model is a simulation environment that comprehensively describes a standardized simulation and evaluation procedure, which consists of plant layout, a simulation model and influent loads including three different disturbances to be used for testing and evaluating the relative effectiveness of different control strategies (Copp, 2002). The simple plant layout consists of five biological reactors (two anoxic reactors and three aerobic reactors) and a settler. The plant is thus capable of achieving simultaneous carbonaceous and nitrogen material removal through nitrification and denitrification. ASM1 (Henze et al., 1987) is used to describe the dynamic behaviour of the biological reactions taking place in the activated sludge process. The double-exponential settling velocity model of Takács et al (1991) is to describe the separation of sludge from treated wastewater. The dynamic inputs to the benchmark model are sampled under three different weather conditions. This is to test and validate the robustness and flexibility of designs with appropriate control strategies. An overview of the benchmark model can be summarized as follows:

**2.4.1 Plant Layout**

The benchmark model configuration (Figure 2.8) consists of five reactors in series, two anoxic reactors followed by three aerobic reactors, and one 10-layer sedimentation tank. The total biological volume is given as 5999 m3. The first two reactors are unaerated but fully mixed and are both assigned volumes of 1000 m3. The remaining three equal-sized vessels are aerobic reactors, each with a volume of 1333 m3. Different values of are assigned for three aerobic reactors as , and . The area of the non-reactive sedimentation tank is given as 1500 m2 with a depth of 4 m. A feed point at the sixth layer from the bottom of the settler is adopted. The recycle scheme in this configuration includes internal and external recycle streams. The internal recycle stream mainly recycles the nitrite generated in the last reactor to the first reactor for denitrification. The corresponding flow rate is given as 55338 m3 d-1. The external recycle stream conveys the activated sludge from the underflow of the secondary settler to the first unit with a default flow rate of 18446 m3 d-1.

1500 m2

1333 m3

1333 m3

1333 m3

1000 m3

1000 m3

18061m3 d-1

55338 m3 d-1

18446 m3 d-1

385 m3 d-1

18446 m3 d-1

**Figure 2.8**Schematic representation of BSM no.1

**2.4.2 Process Model of the Secondary Clarifier**

The process models used in BSM no.1 include ASM1 and the double-exponential settling velocity model. ASM1 describes the biological phenomena taking place in the biological reactors. In spite of ASM1 having several limitations compared to the evolved versions such as ASM2 and ASM3, the IWA group still uses it in BSM no.1 due to its universal appeal and practical verification. A matrix representation has been adopted, which relates state variables to process rate equations in order to represent the stoichiometric relationship between reactants and products (a similar matrix for ASM3 can be found in section 2.3).

Models of sedimentation are based on solids flux theory in which equations are used to represent the relationship between the solids settling velocity and the solids concentration. Generally speaking, the interactions between solid particles result in ‘hindered’ settling whereby an increase in solids concentration causes the settling velocity to decrease. This can be represented by a simple exponential relationship (Figure 2.9) by Vesilind (1968):

where: is the settling velocity in layer (m d-1)

is the max Vesilind settling velocity (m d-1)

is the suspended solids concentration in layer (g m-3)

is the hindered settling parameter (m-3 g-1)

The clarifier is modelled by divided it up into a number of layers with mass balance equations tackling the liquid and solid fluxes between them. In practical clarifiers, however, this effect needs to be tempered by the fact that there is a distribution of particle sizes which varies with height. Smaller particles are more abundant in the higher zones of the clarifier in which the concentration is lowest and so the settling velocity in this region is lower than predicted by the equation above. The double-exponential settling velocity relationship of Takács (Figure 2.9) seeks to address this by specifying the following relationship:

where, the additional variables are:

is the difference between suspended solids concentration in layer and the minimum attainable suspended solids concentration (=).

is the max settling velocity (m d-1)

is the flocculant settling zone parameter (m3 g-1)

**Figure 2.9** Constitutive relationship used in clarifier models

The Takács model (Figure 2.11) in BSM no.1 describes the particulate and soluble compound fluxes in sedimentation tanks (Takács et al., 1991). The tank model is divided into 10 equal-thickness layers with a total depth of 4 m. There is a feed point allocated at the sixth layer from the bottom. The movement of particulate solids in the model is due to both the bulk movement of liquid and the gravity settling of solids. The movement of soluble compounds is only attributed to the bulk movement of liquid. In addition, the velocity of liquid movement can be defined as and respectively. The flux of particulate solids due to the movement of liquid can be thus determined as the product of the concentration of solids in the settler and the bulk velocity of the liquid, expressed as: .

where: is the liquid velocity below the feed layer (m d-1). is the liquid velocity above the feed layer (m d-1). is the cross-section area of the settler, is the flow rate at the bottom layer (m3 d-1) and is the flow rate at the top layer (m3 d-1).

Gravity settling

Bulk Movement

10

9

6

**Feed layer**

2

1

**Bottom layer**

**Figure 2.11** Double-exponential settling velocity model

(Takács et al., 1991)

It should be noted that we decided not to use detailed settling models such as that described above for our optimal designs due to the fact that it would introduce mathematical discontinuities into the model equations which can be problematic during optimization. In addition, we are not concerned with including the design of the settler unit. Since its purpose is to produce clarified effluent and recycle most of the solids fraction, we simply represent this by two parameters, the solids retention time (SRT) and the hydraulic retention time (HRT).

BSM no.1 is defined to be platform-independent. By definition, it should give the same results when implemented using either self-coded or commercial software tools. However, this is not always the case as some of these tools have different specifications of modular units for building models that may result in different model outputs. As a result of further normalization by stipulating the same model equations and modelling procedure, a validated cross-platform benchmark simulation model was created. This substantial effort offers great advantages for researchers who are working on modelling of the activated sludge process.

**2.4.3 Influent Composition and Simulation Procedure**

To test the robustness of the benchmark model configuration, BSM no.1 was simulated subjected to dynamic inputs by COST in co-operation with the second IAWQ task group using a variety of modelling tools (Copp, 2000; Alex et al., 1999; Pons et al., 1999). The time-varying inputs were sampled under three weather conditions, namely: dry weather, rainy weather and stormy weather (Copp, 1999; Vanhooren and Nguyen, 1996). The inputs of each disturbance include 14 days influent data with an interval of 15 minutes, with diurnal variations in inlet flow rate, COD (including , , and ) and nitrogen (, , and ) compounds. Model performance at the extremes of variations in each disturbance is also investigated.

The simulation of BSM no.1 for steady state conditions provides instructive information for design purposes. The simulation of BSM no.1 subject to time-varying inputs investigates the behaviour of time-dependent systems. In addition, BSM no.1 extends the dynamic simulation by another 14 days to show a monthly output trend.

**2.4.4 Performance Evaluation**

To aid the evaluation of the output data determined in the dynamic model simulations, a performance index has been adopted for comparing model responses.The system performance assessment is divided into two levels. The first level concentrates on the analysis of effluent quality, effluent violations and the estimation of operating costs. The second level is concerned with the effect of control strategies on model performance (Alex et al., 2008). We are not interested in this second level, rather we focus on the first level since this performance index is very similar to the variable cost component used in this project. Note that we also add capital costs to our overall Net Present Value, whereas the BSM no.1 design is fixed so capital costs are not considered.

The effluent quality in BSM no.1 is determined using an effluent quality index, which maps the effluent contaminants (such as COD,ef, BOD,ef, TKN,ef and so on) onto a single variable. An example that calculates the effluent quality of the last 7 days of the dynamic simulation under a weather condition is expressed as:

([Vanrolleghem et al., 1996](#_ENREF_54))

where: is the time-varying flow rate and the following time-varying variables are defined as:

where: CODe, BODe and TKNe are the concentrations of suspended solids, nitrate and nitrite nitrogen, , , and the total Kjendal nitrogen in the effluent. , and are the concentrations of particulate COD, heterotrophic biomass, autotrophic biomass, particulate solids and particulate inert in the effluent. and are the concentrations of readily biodegradable COD, soluble inert, ammonia and organic nitrogen in the effluent. is the fraction of biomass leading to particulate products. is the mass of nitrogen per mass of COD in biomass, g N (g COD)-1, is the mass of nitrogen per mass of COD in products from biomass, g N (g COD)-1.

The set of weighting factors converts the pollution components above into pollution units. The values of for pollutions, given by Vanrolleghem et al (1996), represents its relative environmental impact or cost and are summarized in Table 2.5.

**Table 2.5** Weighting factors

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Factor | BSS | BCOD | BTKN | BNO | BBOD5 |
| Value | 2 | 1 | 30 | 10 | 2 |

([Vanrolleghem et al., 1996](#_ENREF_54))

For the effluent violations, some constraints for ammonia, total nitrogen, BOD5, total COD and suspended solids in the effluent are defined and the value of each constraint is summarized in Table 2.6 (This is also treated as the standard for the problems given in chapter 6 of this thesis). An additional methodology is used during simulations to report the number and percentage of effluent violations when the discharged contaminants fail to meet their constraints.

**Table 2.6** Threshold value for each component

|  |  |  |
| --- | --- | --- |
| Component | Threshold value | Unit |
| Ammonium plus ammonia nitrogen | 4 | g N m-3 |
| Total nitrogen | 18 | g N m-3 |
| BOD5 | 10 | g BOD m-3 |
| Total COD | 100 | g COD m-3 |
| Suspended solids | 30 | g SS m-3 |

(Alex et al., 2008)

The details of operating cost functions of BSM no.1 for evaluating process performance will be exclusively discussed in chapter 6 in which we demonstrate a comprehensive analysis of the total plant cost function including investment and operating costs for industrial plants.

The advantage of using a fixed process configuration such as BSM no.1 is that it provides designers a systematic approach to analyze the effect of a variety of control strategies on existing plants and assess the model performance using monetary measurement. The adoption of this method in many applications has significantly reduced the excessive dependence on effluent quality to judge process design.

**2.5 Optimization**

Optimization is a key concept in this research and, in general terms, is the use of specific methods to determine the most cost effective and efficient solution to a problem or design for a process ([Seider et al., 2009](#_ENREF_49)). In this section we carry out a selective review of the following areas:

* Formulation: how diverse engineering problems are mapped onto a single mathematical framework.
* Complexity: what features make optimization problems especially difficult to solve.
* Applications: some uses to which optimization has been put – particularly in the field of chemical engineering.
* Algorithms: the systematic search techniques that are compared on the design problem posed in this work.

Mathematical optimization has been widely used in many applications in the fields of science, engineering and business. It is concerned with developing quantitative expressions (e.g. mathematical models) that allow designers to use mathematical approaches and computer software tools to extract useful information. The formulation of optimization problems for a variety of practical applications has surprisingly similar structure. It is this similarity that enables the development of a methodology that can be used to solve a range of design problems.

Optimization has been applied to chemical engineering applications since the late 1940s and a variety of methods with examples can be found in several excellent texts (Beveridge and Schechter, 1970; Bryson and Ho, 1975; Lapidus and Luus, 1967). Optimization problems are everywhere in chemical engineering arising in process design, process control, model development, process identification and real time optimization. Recent work includes: optimization of chemical process with dependent uncertain parameters (Ostrovsky et al; 2012); optimizing reactors selection and sequencing: minimum cost versus minimum volume (Chebbi, 2014); modelling and optimization for scheduling of chemical batch processes (Qian et al., 2009) and so on. The problems in process design and model development are the major concerns of this work. It is very common that continuous and discrete variables are simultaneously combined in a single problem. Such a problem is referred to as a mixed integer optimization problem. An example of a discrete variable is the decision whether to use a process unit or not which can be modelled as a binary 0-1 variable. In this work we could have specified N (i.e. many) activated sludge compartments and introduce binary variables to allow the optimizer to decide which compartments to use. This, however, as not done in this work since it would have massively increased problem size. Problems only including continuous variables are generally defined as nonlinear programming problems. Over the last two decades, a great number of papers on nonlinear and mixed integer optimization problems in chemical engineering based on different optimization approaches have been published. Some typical examples include: continuous-domain mathematical models for optimal plant layout (Papageorgiou and Rotstein, 1998); the optimal design of membrane systems (Marriott and Sørensen, 2003); systematic network synthesis and design-problem formulation, superstructure generation, data management and solution (Quaglia et al., 2014) and so on. In general these problems are very challenging and simplifications have to be made to render them tractable. Even then, provably optimal solutions are rare.

In general, the aim of optimization in wastewater treatment plants is to yield a cost effective treatment for a variety of wastewater compositions. Due to the importance of biological wastewater treatment processes and a great number of existing facilities, there has been a considerable amount of research dedicated to the use of optimization combined with mathematical modelling to improve the design and performance of wastewater treatment plants. Some of representative contributions are: the selection of operational strategies in the activated sludge process based on optimization algorithms (Ayesa et al., 1998); the optimization of activated sludge reactor configuration: kinetic considerations (Scuras et al., 2001); optimal policies for activated sludge treatment systems with multi effluent stream generation (Gouveia and Pinto, 2000); the application of mathematical tools to improve the design and operation of activated sludge plants (Rivas et al., 2001). However, all of this effort only focused on optimization based on static models and overlooked a fact that wastewater treatment plants are inherently dynamic due to the varying flow and loads. The optimal designs determined were only suitable for incoming wastewater with a constant flow rate. Such designs in practice might perform poorly in dealing with varying inputs (both flow rate and compositions).

**2.5.1 Formulation of Optimization Problems**

Every optimization problem consists of the following components:

* A set of variables
* An objective function
* Equality constraints (equations)
* Inequality constraints (inequalities)
* Lower and upper bounds on some or all of the variables ([Seider et al., 2009](#_ENREF_49))

A general form for optimization problems is displayed as follows:

Minimize/maximize:

Subject to :

(Edgar et al, 2001)

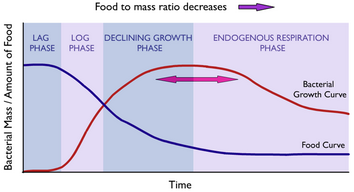
where: is a vector of n variables (…., ). is a vector of equations and is a vector of inequalities.

Equality constraints are usually defined as process model expressions. They describe the chemical, physical and biological behaviour of process. The role of inequality constraints is to define a feasible region for the selection of optimal solutions. The constraints could include simple upper and lower bounds on variables. The solutions determined that satisfy all the above restrictions while maximizing or minimizing the objective function over a given domain, are treated as local/global optimal solutions. The objective function for industrial applications is commonly expressed in monetary units since the major objective of enterprises is to maximize profit or minimize costs. For example, the objective of this study is to yield an optimal design for wastewater treatment plants at a minimum cost while meeting the effluent discharge standards.

Numerous optimization methods (e.g. numerical and heuristic search algorithms) have been developed during the last few decades. The rapid progress in computer technology makes these methods more efficient for searching optimal solutions. Choosing an appropriate method for any particular cases, however, is a complicated step. It depends very much on the nature of the problems and the characteristics of the objective functions as well as the number of dependent and independent variables. A challenging feature of optimization problems is their unpredictability. Sometimes one algorithm can perform well, whereas another completely fails to find any solution at all (Edgar et al.,2001). In this work, the complexity of the process considered means that we have sought to avoid the introduction of discrete or binary variables. Instead we use continuous cost curves to represent the economies of scale for capital costs. Below we emphasize some of the challenges of tackling continuous problems.

**2.5.2 Challenging Features of Engineering Optimization Problems**

The optimization problems encountered in engineering applications can be classified into two categories, linear and nonlinear, with the latter being far more difficult to solve. The design problems in wastewater treatment plants, like many others, behave in a nonlinear fashion. A simple example that represents such a nonlinear behaviour is the microorganism growth in a batch culture in Figure 2.12, although it only partially reflects the real behaviour of the biological processes in wastewater treatment plants. It can be seen that the metabolism of the bacteria in the batch reactor are nonlinear with respect to the concentration of substrate (e.g. COD and BOD) as well as time. The growth of the micro-organisms starts from the acclimatization and then goes through an acceleration phase in which the amount of biomass increases exponentially within a short generation time. However, the trend reverses and goes down dramatically when the substrate becomes limited. It should be noted that, although most problems are nonlinear, it is still possible to solve them using locally linear methods employed in an iterative manner, such as sequential linear programming (Wilkinson et al., 2008). Indeed, this is one of the approaches used in this work.



**Figure 2.12** Microbial growth curve (EBS, 2013)

As mentioned earlier, linear programming, nonlinear problems are inherently difficult to optimize due to their unpredictable behaviour, even with the advent of high-speed computers. The presence of constraints adds another level of problem complexity. Those problems having one or more equality and inequality constraints are referred to as constrained optimization. In this work, for example, a key set of constraints are the material balance equality constraints linking each process compartment. It is worth listing a number of difficulties when solving such constrained, nonlinear problems below:

* Local/global optimum

It is very difficult to differentiate a local optimum from a global one.

* Multiple disconnected feasible regions

In the presence of nonlinear constraints with complex characteristics, several different feasible regions providing optimal solutions could exist but be unconnected. The search for a global optimum covering all possible regions would be time-consuming.

* Starting point

Different starting points may lead to different optimal solutions due to the multimodal feature of objective functions.

* Algorithm selection

Choosing an appropriate optimization algorithm *a priori* from numerous methods for a specific problem is difficult. The trade-off between accuracy and computational effort should be considered. (Seider et al., 2009)

**2.5.3 Analytical vs. Numerical Methods**

Analytical methods, prior to the computer era, were the main method for optimization. In this work we use the analytical method of Harmand et al (2003, 2004, and 2005) to compare the performance of a range of numerical methods. For the unconstrained case, it is based on deriving expressions for the derivative of the objective function and then making them equal to zero to determine the optimal solution. For the constrained case, the derivatives of the constraints are also required to conform to a set of conditions called the Karush-Kuhn-Tucker conditions at optimality. If constraints are active then the gradient of the objective function will be non-zero at optimality. However, analytical techniques are strongly limited and only tend to be used for cases where nonlinear objective functions have one or twovariables. Analytical solutions for problems having several dependent variables (e.g. more than 5) do not exist, unless for simple unconstrained examples. Therefore, most researchers shift their preferences to the use of numerical methods to solve more complex optimization problems.

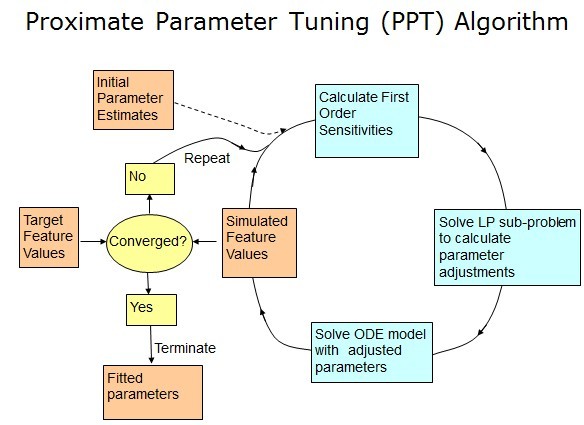
Examples of iterative numerical techniques, similar in principle to those employed in this work include Newton and Quasi-Newton methods and polynomial approximation methods. The principle of these techniques is to iteratively evaluate the values of the functions by successively narrowing down a bracket of minimum expressed as an interval. As long as the bracket is sufficiently reduced, the minimum is considered to be at the center of that interval ([Antoniou and Lu, 2007](#_ENREF_5)). Apart from these methods, some others depending solely on function evaluation also can achieve model optimization. They are random search, grid search, univariate search and simple search method(Seider et al., 2009). These methods are very simple to understand and are commonly preferred when dealing with objective functions with non-smooth characteristics.

Multidimensional unconstrained problems are the other class of nonlinear optimization problems. The method of steepest descent, evolved based on the line search method, is commonly used for unconstrained problems with a number of variables. It is an iterative procedure to locate the local minimum of functions by conducting a line search strategy to the computed descent direction. This process repeats until some necessary conditions are met. In addition, other methods dealing with multivariable constrained problems include successive linear programming, successive quadratic programming and the generalized reduced gradient method. A more detailed description for the nonlinear programming can be found in Edgar et al (2001).

**2.5.4 Optimization Methods in Sentero and Copasi**

As was mentioned, the aim of this work is to address the simultaneous optimization of the system structure and operating conditions of wastewater treatment plants to yield a cost effective design for a variety of compositions. To do this, some available numerical optimization methods and heuristic search algorithms in Sentero and BioWin are applied and implemented to solve the process synthesis problems in chapter 4-6. A brief introduction of these methods is given as follows:

First, the proximate parameter tuning algorithm (PPT) in Sentero is introduced (Wilkinson et al., 2008). Similar to Newton’s method, it utilizes the gradient method to calculate the first order sensitivities of required model output features with respect to each parameter in order to calculate new parameter values that can shorten the distance between the real target features and the nominal model outputs. This algorithm searches for new parameters in an iterative manner with a certain step length and stops when the maximum number of iterations or the optimum criterion is achieved. The schematic diagram of the PPT algorithm is below displayed

**Figure 2.13** Proximate Parameter Tuning Algorithm

(Wilkinson et al., 2008)

This method is used in chapter 4 to determine the optimal design parameters of a minimum WWTP model.

The optimization algorithms in Copasi implemented in this work include Levenberg-Marquart, random search, evolutionary algorithm, simulated annealing and particle swarm (Videolectures, 2013; Gentle et al., 2012; Fouskakis & Draper, 2002; Collet, 2006). These algorithms are further classified in two categories: numerical and heuristic search algorithms. More details of these optimization approaches are given as follows:

* Levenberg-Marquardt

Levenberg-Marquardt is a mathematical optimization method that combines the Gauss-Newton algorithm and the gradient descent method. Using this method, the minimum of a multivariable function can be determined and navigated no matter how far the current solution is away the best one (Lourakis, 2005). This method has been widely used for solving the nonlinear least-squares problems, which arise from fitting the parameterized function to a number of meaningful data by minimizing the sum of the squared error of residuals between functions and data (Gavin, 2011)**.** It utilizes a curve-fitting method to update new parameters in the direction of the reduced least squares objective when the parameters are far from the optimal solutions. It also treats functions as quadratic functions as to estimate the optimal solutions through an approximation when the parameter values are close to their optimal values.

* Random search

Random search is one of the most widely used numerical optimization methods. It does not require the calculation of gradient to search for optimal solutions within a continuous domain. Functions to be solved using this algorithm can be either continuous or discontinuous. This method iteratively locates the best solutions for a given objective problem in a search space that has been selected from a certain range surrounding the current solution. This method is quite useful for the estimation of the location of roots or optima. However, some further refinement by numerical techniques is required (Cooper and Steinberg, 1970).

* Evolutionary algorithm

An evolutionary algorithm is a heuristic optimization algorithm using approaches inspired by behaviour of evolution found in nature to find an optimal solution for a given problem. There are a variety of evolutionary algorithms (e.g. genetic algorithm, evolutionary programming, genetic programming and classifier systems) that have been widely in many applications in the fields of science and engineering. All of these methods are based on the same underlying principle that the objects to be modelled are treated as an ecosystem. With given a population of individuals, the ecosystem forces a population of individuals to produce generations. This improves the fitness of individuals (Eiben and Smith, 2010). With given a set of candidate solutions, this algorithm eliminates the individuals with lower fitness and keeps others seeding the next generation by applying recombination and mutation. Two or more selected candidates (the so-called parents) are combined into one or more new candidates (the children). This is the purpose of the recombination. Mutation is for the conversion of an old candidate to a new one. By executing the two processes, a set of new candidates (the offspring) with high fitness will be finally selected through a competition (Deb, 2001). A flow sheet that represents an evolutionary algorithm is given as follows:

Initialization

Parents

Recombination & Mutation

Population

Termination

Offspring

**Figure 2.14** The general scheme of an evolutionary Algorithm

(Eiben and Smith, 2010)

Although most evolutionary algorithms have similar techniques, they differ from each other in details. For example: the genetic algorithm seeks the solution of a problem in the form of strings of numbers by applying recombination and mutation. It is commonly used for solving optimization problems. The evolutionary programming is similar to the genetic algorithm, but the structure of the program is fixed and its numerical parameters are allowed to evolve.

* Simulated annealing

Simulated annealing is a probabilistic method proposed byKirkpatrick et al (1983) and Černý (1985) to iteratively determine the global minimum from a number of local minima. In fact, it models a physical process where a solid is gradually heating up and is then slowly cooling down.

A new point (a minimum point) that lowers the objective of the process is generated in each iteration when the solid is cooled slowly with the temperature held steady at a series of levels long enough for the solid to reach thermal equilibrium with its environment. It also keeps a distance between the new and the current points by a probability distribution with a scale proportional to temperature(MathWorks, 2013).

* Particle swam

Particle swarm is a population-based stochastic approach for solving continuous and discrete optimization problems (Dorigo et al, 2008). Inspired by the behaviour of flocking bird, each particle has a velocity when it moves in the search space with the aim of searching for the optimum value of a specified objective. Particles also remember the positions they were in for good candidate solutions to the optimization problem found previously. As the particles co-operate, during the search, they exchange the information about what they have discovered in the places they have visited. On receiving such information about better positions from its neighbour, a particle will immediately move towards it with an adjusted velocity. The new position it will take is the sum of its old position and the new velocity. By appropriately defining the particle velocity and population size, it may facilitate the search for the optimal solutions.

**2.6 Process Synthesis**

For engineers, the term process synthesis means to translate new academic discoveries into a process flowsheet and a base-case design. This concept was proposed half a century ago by Rudd and his students (Siirola et al., 1971; Siirola and Rudd, 1971; Powers, 1972). It primarily focused on the development of a functional process system including a variety of process operations which are capable of achieving a desired task ([Nishida et al., 1981](#_ENREF_42)). These operations include the conversion of raw material into new products and the separation of multi-component mixtures. The concern of other aspects (e.g. providing a safe operating environment, maximizing potential profits, maximizing production rate and so on) did not draw much attention. Taking such aspects into consideration, a number of promising approaches were developed in the later twenty years. These approaches can be classified into two types: hierarchical decomposition approaches including rules of thumb or heuristics (Douglas, 1988) and algorithmic methods using mathematical programming theories (Grossmann, 1985, 1989, 1990).

Synthesis problems in engineering applications are sometimes solved by hierarchical decomposition approaches using a sequential decomposition strategy. Breaking down problems into a hierarchy of decisions, the potential solutions at each decision level are determined, analyzed and evaluated. A number of alternative designs are thus formed as a result of exploring new decisions on process flowsheets. However, due to the sequential nature of decisions ignoring the interactions between decisions in different decomposition levels often leads to sub-optimal solutions (Yeomans and Grossmann, 1999).

Since they are capable of simultaneously optimizing process synthesis problems, algorithmic methods based on mathematical programming techniques (i.e. Mixed-Integer Nonlinear Programming) have been widely used in many industrial applications. The approaches complement the defects of hierarchical decomposition methods, allowing interactions between system components. This increases the possibility to determine near-optimal or even optimal solutions (Daichendt and Grossmann, 1998). A typical example of using such approaches for wastewater treatment applications is by Mussati et al (2005), who proposed a superstructure representation and a MINLP models for the simultaneous optimization of process configuration and operating conditions of activated sludge plants.

Other studies addressing process synthesis in wastewater treatment plants based on heuristic optimization approaches have also been reported over the past 10 years. Rigopoulos & Linke (2002) applied heuristic optimization approaches in the form of simulated annealing to a superstructure model of the activated sludge process to search for optimal solutions in order to meet target performance. They suggested that the use of mathematical programming in the form of MINLPs for the highly nonlinear and discrete nature of synthesis problems extracted from the superstructure should be restricted to search for local improvements, whereas a heuristic optimization algorithm used was used to find globally good solutions. Other examples of using heuristic algorithms to solve the similar synthesis problems include: Balku and Berber (2006) who used an evolutionary algorithm to solve the aeration schedule optimization problem in the activated sludge process to minimize the energy consumption due to the aeration. Kusiak & Wei (2012) employed the particle swarm algorithm to a multi-objective model of the activated sludge process to maximize the effluent quality while minimizing the energy consumption.

In this study, we mainly use a heuristic optimization algorithm in the form of particle swarm to solve the process synthesis problems in wastewater treatment plants. In contrast to the examples just delivered, we tackle the complexity of dynamic inputs but save on the complexity of having discrete variables (we consider that the tractability of mathematical programming techniques for such complexity is under question). The objective to be achieved in this research is to ensure a good effluent quality at a minimum cost. The level of decision making for the general process synthesis for activated sludge plants are summarized into the following sequential steps:

* Batch or continuous

Treating the large amounts of influent wastewater, continuous processing units are selected.

* Input-output structure of the flowsheet

It is important to identify the characteristics of incoming raw material to systems and verify the specifications of desired products before formulating process flowsheets. This provides designers instructive information and leads them to choose appropriate equipment. The equipment used in chemical engineering based on distinct functionalities is classified into a number of types in which the most representative ones are distillation columns, absorbers, strippers, evaporators, heat exchangers, bioreactors, sedimentation and so on. Biological reactor and sedimentation tank are the key components in the activated sludge process.

Feed

(COD & SNH4)

Purified effluent

Wastewater treatment process

Streams

**Figure 2.15** Input-output structure

* Process flowsheet determination

Having identified the specifications of desired products, the characteristics of selected equipment and interconnecting streams, the synthesized process flowsheet of the conventional activated sludge process is displayed in Figure 2.16. The process consists of a bioreactor and a sedimentation tank. The biodegradable COD and nitrogen material feeding to the process are expected to be removed due to the microbiological activities in the reactor. Such conversion processes are usually based on the reaction of electron transfers, free-radical exchanges and other reaction mechanisms. The formulation of the overall material balance equations is also done at this stage.

Reactor

Separation

Feed

**Figure 2.16** Simple process flowsheet

* Simulation and optimization

Simulators are software tools that allow designers to build, solve and analyze mechanistic models using a number of solvers. Simulation is a key component in process synthesis as it checks whether the synthesized process yields reasonable products with similar specifications as the desired ones and also evaluates the behaviour of processes. Biology software tools are applicable to the activated sludge process to evaluate the behaviour of biological reactions in the steady state by solving material or energy balance equations. The objective of the activated sludge process model is to eliminate COD and nitrogen matter in the process and yield clean effluents that meet discharge standards. Depending on the quality of simulation results, designer/modellers can decide whether to apply optimization or whether to retain the original process structure.

In this work we use heuristic optimization approaches for stages 3 and 4 to determine optimal designs for more complex wastewater treatment plants. The detailed method to achieve such an objective is given in the next chapter.

**2.7 Summary**

In this chapter, the activated sludge and the anaerobic digestion processes are presented. Both have shown their abilities to degrade COD and nitrogen in municipal and industrial wastewater with a high removal rate. However, different shortcomings of their evolved configurations are also addressed as these designs that are mainly based on empirical knowledge or pilot plants yield high operating costs. It is thus decided to adopt mathematical modelling to investigate the details of internal cause-effect relationship within processes, thus evaluating the impact of design parameters/variables on model output features. The subsequent introduction of optimization methods coupled with mathematic modelling allows the automating search for the best design candidates from a variety of parameter combinations to achieve the dual wastewater treatment objectives of minimum total cost and low effluent compositions.

1. **Method**

The method used in this thesis is divided into two parts, modelling and optimization. In the first part we focus on modelling of wastewater treatment plants. Using modelling approaches can translate the physical, chemical and biological aspects of processes into the form of amenable mathematical equations. These mathematical expressions include, for example, the dynamic balance equations describing reaction kinetics and reactor hydraulics. Numerical integration methods can then be employed to solve these differential equations in order to determine the profile of each species over time in a controlled volume of reactor. The second part is dedicated to seeking to improve the design and performance of wastewater treatment plants using a variety of optimization approaches in Copasi. Unlike traditional design approaches based on averaged inputs, we aim to develop a novel one that takes dynamic variations in both feed compositions and flow rate into consideration as a part of optimization. A further comparison between the traditional and our novel approaches will be presented and discussed in Chapter 6.

To facilitate the understanding of the dynamic behaviour of bacterial growth in wastewater treatment processes and provide a basis for evaluating a range of optimization algorithms, a simple motivating example considered as a minimal model of wastewater treatment plant is structured and simulated in chapter 4. Modelling of an industrial wastewater treatment plant using several simulation software tools is carried out in chapter 5 and chapter 6 respectively. The modelling method is here summarized into five steps:

* Synthesis of Unit Connectivity

Since we concentrate on the modelling of biological treatment processes, the physical process design of the preliminary treatment stages (such as the design of the primary processes for the removal of gross solids and grit) is not considered in this work. For this work we consider a flowsheet (Figure 3.1) consisting of three CSTRs in series and a sedimentation tank. This process configuration is treated as an evolved version of the conventional activated sludge process. Constraining the final process design a maximum of three CSTRs is a decision that is made necessary by the complexity of the dynamic optimization problem we are tackling. The minimum number to achieve reduction of both COD and total nitrogen is two since at least one aerobic reactor and one anoxic reactor are required. More generally, it has found that CSTRs in series can greatly save total required tank volume (Hill and Robinson, 1989).This configuration allows the investigation of the possible benefit of using a distributed feeding system and a recycle stream. The sedimentation tank allocated at the tail end of the flowsheet aims to separate the mixed liquor suspended solids generated in the last reactor into clean effluent and sludge. As discussed in the previous chapter (section 2.4), we assume that there is a perfect separation in this process. Some sludge from the settler is recycled back to the first reactor with a flow rate of . The parameter is treated as a key decision variable in the optimizer and is in a range of 0 to 30 – i.e. several multiples of the external flows can be recirculated internally. The remaining sludge (a much smaller fraction) is treated as waste and removed from the system. In steady state, the wasted sludge balances the overall generation of sludge in all the reactors produced by growth of the microorganisms. The aim of the recycled sludge is to ensure sufficient amounts of biomass remaining in the first reactor for COD degradation

Feed

Unit 1

Unit 2

Unit 3

Effluent

Recycle stream

Settler

Waste sludge

**Figure 3.1** Flowsheet of the activated sludge process

* Process Model Design

Choosing appropriate models that sufficiently represent the physical, chemical and biological behaviour of wastewater treatment processes is of prime importance.

The term wastewater treatment plant model, by definition, is an ensemble of activated sludge process model, hydraulic model, oxygen transfer model and settler model so that a complete wastewater treatment plant can be fully represented. Wastewater treatment plant models consider both aspects of conversion and transport processes, the former of which are associated with the biological reactions taking place in processes and are independent of the type of reactor and the size of reactor. ASM3 is used to represent the conversion processes in this work. The transport processes, on the other hand, are characteristic for the design of physical systems. These processes describe tank volume, hydraulic tank behaviour and flow rate (such as internal and external recycle flow rates). All these defined processes are finally summarized in the form of balance equations.

The balance equations are the combination of the mixing and the mass transfer characteristics of each individual reactor compartment. Therefore, the equation for each species should couple concentrations and flow rates in the links between compartments. An example of this (Equation 3.1) is the general mass balance equation for soluble or particulate components when continuous stirred tank reactors are employed:

where: is the control volume of the compartment unit; is the volumetric flow rate entering and leaving the compartment; is the influent concentration of the component ;and is the reactor concentration of the component . As was previously mentioned in process kinetics section in chapter 2, the system reaction term () is the sum of the products of the stoichiometric coefficient and the process rate expression for the component . The detailed information of stoichiometry and process rate equations of ASM3 can be found in Table 2.3 and Table 2.4.

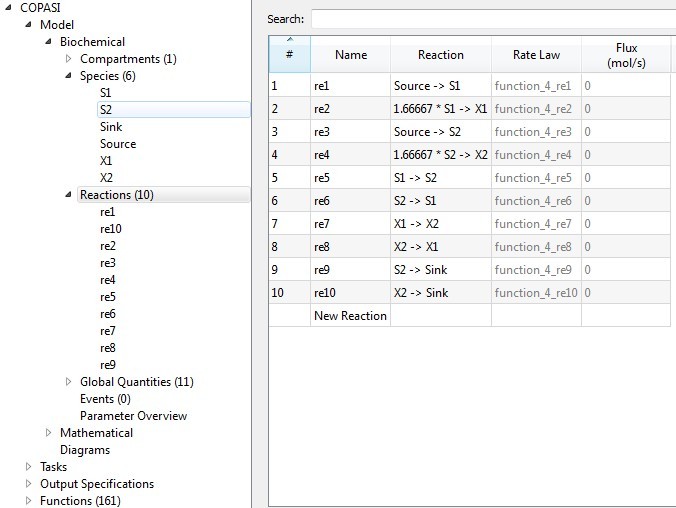
The formulation of the balance equation for any gaseous phase products in processes is slightly different as it considers the rate of liquid-gas mass transfer for a soluble gas, which is characterized by the value of parameter a. An example describing the mass transfer of the dissolved oxygen between the gas and liquid phases in processes can be expressed as:

where: is dissolved oxygen concentration; is oxygen saturation constant at 15oC; is the dissolved oxygen concentration in the effluent; and is the liquid side dissolved oxygen transfer coefficient.

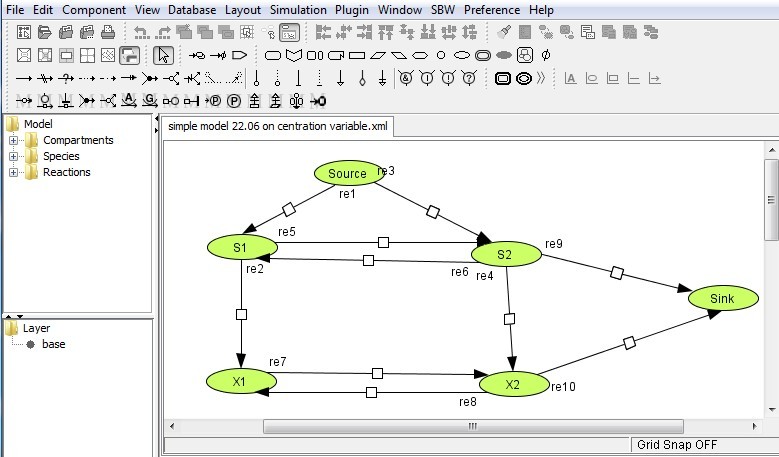
* Model Development in Different Simulator Environments

Since we defined the wastewater treatment plant model in the form of differential equations, we choose four kinetic simulator software tools: CellDesigner ([http://www.celldesigner.org](http://www.celldesigner.org/)), Copasi ([http://www.copasi.org](http://www.copasi.org/)), BioWin (<http://envirosim.com/>) and Sentero (<https://www.sheffield.ac.uk/polopoly_fs/1.48155!/file/Sentero.pdf>), to solve the synthesis problems in this work. In terms of functionality, we also compare and contrast the analytical capability and the user interface between these tools. A detailed discussion is given as follows:

User interface is a key function in the determination of model definition in simulators. There are two major types: the dialog box interface and the diagrammatic interface. For example, models in Copasi are defined through the dialog box interface (Figure 3.2) in which there is no need to explicitly write kinetic equations. It is only necessary to input the specific reactions and reaction rate expressions with defined parameters. This provides an indication of which compartment the reactions are confined to. However, the visualization of the network configuration is not available using the dialog box interface. The diagrammatic interface (Figure 3.3) used in CellDesigner, Sentero and BioWin complements the above defect as it enables modellers to draw diagrams rather than coding equations. Rate expressions and parameter values can be added to models by double clicking the corresponding objects in diagrams (Funahashi et al., 2003). There is a common feature existing among these four simulators that a predefined library of rate expressions for various metabolism reactions is provided. This simplifies the model construction in some cases. Figure 3.2 displays a minimal model defined in Copasi. Figure 3.3 shows the network of the minimal model in CellDesigner. Table 3.1 shows a comparison of the features between dialog box and diagrammatic user interfaces.



**Figure 3.2** A simple model defined in Copasi



**Figure 3.3** Diagrammatic interface of CellDesigner

**Table 3.1** Dialog box and diagrammatic user interfaces

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Type of software | Program | Type of interface | GORM\* | ROIRRTI\* | LOPRX\* | ELOAPC\* | AAFANL\* |
| SAS\* | CellDesigner | D\* | Yes | Yes | Yes | NA | Yes |
| Sentero | D\* | Yes | Yes | Yes | Yes | NA |
| Copasi | DB\* | NA | NA | Yes | Yes | NA |
| BioWin | D\* | Yes | Yes | Yes | NA | NA |

([Alves et al., 2006](#_ENREF_4))

(Abb: SAS\*: stand-alone simulator; D\*:diagrammatic; DB\*: diolag box; GORM: graphic of representation multiple compartments; ROIRRTI\*: representation of interface reaction, reactant types and interaction; LOPRX\*: library of predefined rate expressions; ELOAPC\*: editable lists of all parameter conditions; AAFANL\*: alternative algorithms for automated network layout)

The core functionality of all simulators is the ability to numerically solve large systems of ordinary differential equations (ODEs) as illustrated in Table 3.2. The ability to specify and solve partial differential equations that might be required to model, for example, spatial effects, are absent from all of the simulators. Instead, spatial effects can be approximated using compartments assuming that spatial heterogeneities within compartments are neglected. The ability to perform stochastic simulations is only available in Copasi. The stochastic modelling approach treats molecules as discrete entities with productive molecular collisions occurring at discrete events in time. Such modelling, however, is not of interest in this work. It is computationally intensive and applicable to modelling low copy number proteins and mRNA within cells.

Another specialized functionality for the analysis of dynamic models is the ability to produce a steady state solution to the set of ODEs. This is done by setting the left hand side accumulation terms to zero and finding a solution to the resulting non-linear algebraic equation set. This is offered only by Sentero and Copasi, allowing steady state sensitivity analysis to be performed. Another feature, only offered by Sentero is time-dependent sensitivity analysis in which, for example, the sensitivity of the height of peak value of species concentration to each parameter can be automatically calculated.

Finally, a capability which is of deep interest in this work is the ability to perform optimization whether as part of a parameter estimation routine or standalone. The user is able to specify an objective function made up of outputs from the model simulation and optimize it by varying key parameters. Only Sentero and Copasi can be used for this work with Copasi having the advantage that it offers a range of alternative algorithms.

**Table 3.2** Analytical capabilities of each simulator

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Type of software | Program | ODE | Partial differential equation | Stochastic | Steady state sensitivity analysis | Time-dependent sensitivity analysis | Parameter estimation/ optimization |
| SAS\* | CellDesigner | Yes | NA | NA | NA | NA | NA |
| Sentero | Yes | NA | NA | Yes | Yes | Yes |
| Copasi | Yes | NA | Yes | Yes | NA | Yes |
| BioWin | Yes | NA | NA | NA | NA | NA |

([Alves et al., 2006](#_ENREF_4))

(SAS\*: stand-alone simulator)

CellDesigner, providing intuitive networks for processes to be modelled, is considered as the optimal choice when only kinetics modelling is required. BioWin, the commercial WWTP software tool, is employed for a case study presented in chapter 5 in order to retrofit a wastewater treatment plant in China. Sentero, is used to deal with the process synthesis of a minimal wastewater treatment model given in chapter 4. Among four simulators, Copasi is the only one that has both deterministic and stochastic optimization algorithms. The latter algorithms can be highly efficient in finding near-optimal solutions to the intractable nonlinear programming problems with many degrees of free. It is mainly employed in chapter 6 to solve the nonlinear programming in an industrial wastewater treatment plant.

Model cross-compatibility, is another significant aspect that we consider during model construction. Coding our models in System Biology Markup Language (SBML) ([Hucka et al., 2003](#_ENREF_35))can make models more compatible so that they can be freely shared between other communities/tools.

* Mapping A Systems Biology Tool to Process Synthesis Problems

Using Copasi as the major tool to construct and optimize the multi-compartmental models in chapter 6, presents a few challenges that needed to be addressed. Some of these relate to the fact that Copasi was not designed to model the bulk transfer of material from one process unit (or compartment) to another. Copasi works with species concentrations at the state variables but, for inter-unit transfer we needed to work in units of absolute mass. Our state variables therefore relate to the absolute mass of each species in each compartment and, where a species participates in a reaction, we need to use the mass divided by the compartment volume each time the concentration is required. Another issue that it was necessary to address arises from the fact that Copasi does not allow the process stoichiometry or compartmental volumes to be parameterized and therefore adjusted by the optimizer. This is a problem when the key decision variables in our optimization ( and ) relate to the stoichiometry of the flow between the process units, or the volume of those units. This problem was solved by having all stoichiometry values set to their default values of unity and subsuming the decision variables into pseudo reactions representing the bulk transfers between process units. Another problem is that the optimizer in Copasi can only use values of the variables at the final time of simulation. In our dynamic model, however, we consider the time-varying inputs and outputs over a year and therefore time-varying operational costs which must be accounted for. In chapter 6, therefore, we formulate a dummy reaction that accumulates the daily costs to a total value and it is this end-of-horizon value that is used in the objective function for the optimization.

* Validation

We validate our modelling methodology by replicating a published model and then make a comparison of the process outcomes between two models. The model by Alasino is chosen as the basis to compare so that our model should have the same configuration. The essential design parameters, the input compositions and the operating conditions in our model simulation are also consistent with Alasino’s. The detailed information of the validation is presented in part I of chapter 6.

In the second part, we seek to improve the design and the performance of WWTP models using a variety of optimization approaches in Copasi. Unlike previous attempts which focus on the optimal design of wastewater treatment plants subject to averaged inputs (steady state), we take the dynamic variations in both feed compositions and flow rate into consideration as a part of model optimization. However, due to the highly combinatorial and nonlinear nature of synthesis problems in the dynamic models, we apply the particle swarm algorithm, rather than mathematical programming approaches, to keep problem complexity under control. A systematic comparison between the optimal designs determined under the steady state and the dynamic conditions is also carried out. The scheme of this methodology procedure is illustrated in Figure 3.4.

Model initialization

(Process model chosen)

Simulator environment selection

Model simulation

Validation

Optimization

**No**

**Yes**

Steady state model optimization subject to averaged input

Dynamic model optimization subject to time-varying inputs

Selection of the best design solution

**Figure 3.4** Research methodology

1. **Validating Our Approach Using a Simple Analytical Example**

**4.1 Preface**

In this chapter, we present a simple motivating example considered as a minimal model of the activated sludge process describing organic carbon degradation. The advantage of this example is that it is amenable to solutions by analytical methods. This enables a direct comparison with numerical optimization methods. We determine the optimal designs for the simple model given in Figure 4.1 using the extensive suite of numerical and heuristic optimization algorithms provided in Copasi and Sentero in order to reach the maximum substrate removal rate or the minimum total required reactor volume. This effort also facilitates the understanding of the mechanism of bacteria growth in wastewater treatment processes as well as evaluating a range of optimization algorithms that can be applied to the more complex problems as discussed in chapter 6.

**4.2 Simple Model Formulation (Two CSTRs in Series)**

Reactor 1

()

Reactor 2

()

Recycle loop,

**Figure 4.1** Flowsheet of the simple model

(Harmand et al., 2003, 2004 and 2005)

Figure 4.1 shows that the model consists of two CSTRs in series; (represented by ) and (represented by ) are the two streams distributed from the total inlet flow () feeding to the two reactors () respectively. A recycle stream () from the second reactor to the first one is also considered. For each reactor, the model deals with two state variables () based on the Monod kinetics. and are the concentrations of biomass and substrate in the first and second reactors respectively. is the feed substrate concentration. The main drive to simulate such a simple model is that it is considered sufficient for a good dynamic description for the substrate degradation process. This would avoid consuming much time on the investigation of dynamic behaviour using more complex processes. The major parameters used in this model include the hydraulic retention time (determined by ), the coefficient of inlet flow rate () and the coefficient of recycle flow rate ().

According to the flowsheet given in Figure 4.1, the mass balance equations expressing the substrate utilization and the biomass growth in the model are displayed as follows:

(4.1)

The left hand sides of these ordinary differential equations are zero when the system is at steady state. The values of parameters to be used in the model design are listed in Table 4.1

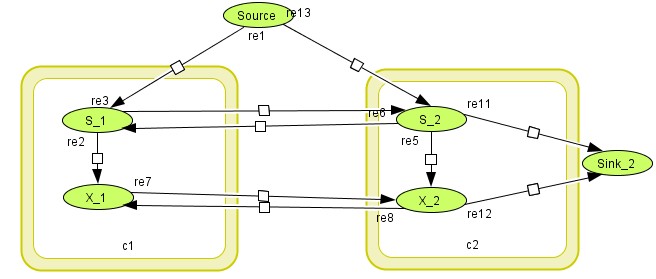
**Table 4.1** Parameters used in the mode construction

|  |  |  |
| --- | --- | --- |
| Parameters | Value | Unit |
| Total inlet flow rate | 1000 | m3 d-1 |
| Total inlet substrate concentration | 300 | g COD m-3 |
|  | 0-1 | - |
|  | >=0 | - |
| Max specific growth rate | 3 | d-1 |
| Utilization rate | 0.67 | g cell per g COD |
| Half-saturation coefficient () | 20 | g COD m-3 |
| Volume of the first reactor () | 660 | m3 |
| Volume of the second reactor () | 550 | m3 |

The total inlet flow rate is given as 1000 m3 d-1 and the inlet substrate concentration as 300 g COD m-3. , as the specific growth rate, is set as 3 d-1 and , the biomass yield from substrate, is defined as 0.67 g cell per g COD. , the half-saturation coefficient, is given as 20 g COD m-3. The volume of the first reactor is given as 660 m3 and the second reactor as 550 m3. is the coefficient of inlet flow rate varying from 0-1. , the coefficient of recycle flow rate, is defined as an arbitrary positive value.

**4.3 Model Simulation in CellDesigner**

The simple model based on the process kinetics shown in the specified mass balance equations and the nominal parameters given in Table 4.1, is structured in CellDesigner. The network of the model is displayed in Figure 4.2.

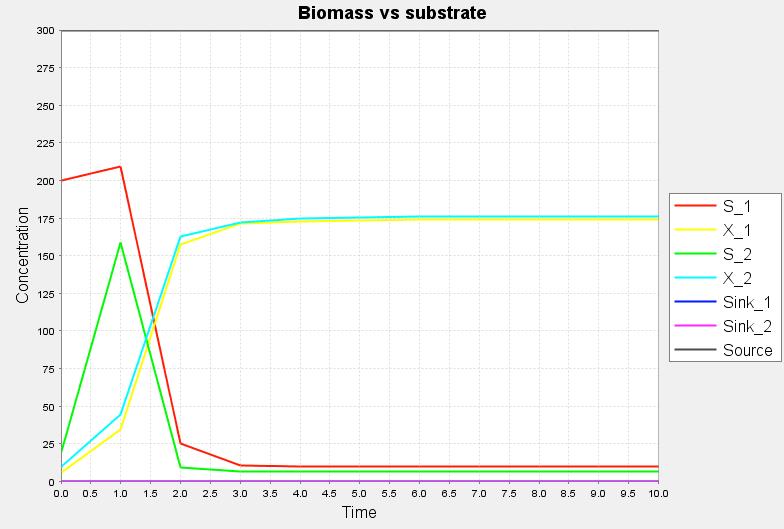


**Figure 4.2** Simple motivating model

It can be seen that the model shown in Figure 4.2 is the duplicate of what is given in the process flowsheet but with different symbols representing each component. The substrate () from *Source* is fed to the two compartments () through two separate streams. A single reaction occurs in each reactor in which the substrate () is converted into the biomass (). Material transfer between the two reactors is considered. This ensures a secondary degradation in the second reactor if large amounts of untreated substrate leave the first unit. Some generated biomass from the second reactor is also recycled to the first unit in order to maintain sufficient amount of bacteria for substrate degradation.

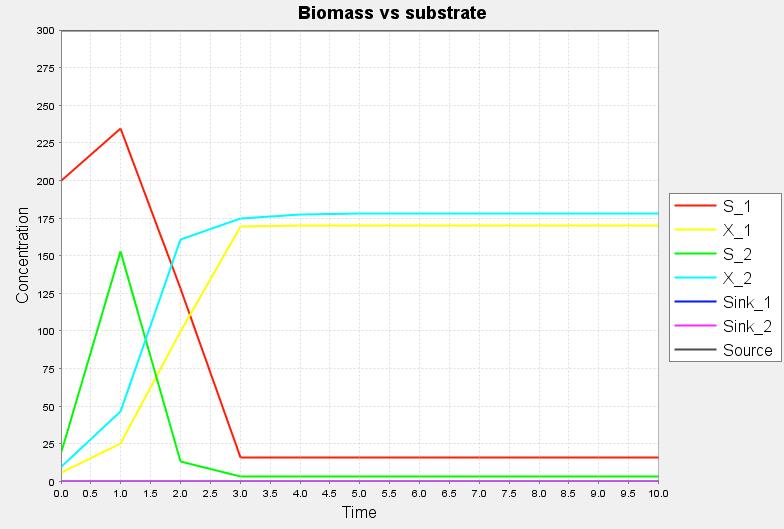
To investigate the effect of distributed feeds and recycle streams on substrate removal and bacteria growth, the model with different combinations of nominal parameters (referring to  *&* ) was simulated and the corresponding outcomes are separately shown in the following figures. This, in a sense, evaluates the design parameters and attempts to improve the model performance through a trial-and-error fashion.

Figure 4.3 illustrates the model performance in terms of biomass growth and substrate degradation when is set as 0.6 and as 0 (which means no recirculation is required). There is a significant decrease in the concentration of substrate () in the second reactor from 155 to 8 g COD m-3 due to the rapid rise in the production of biomass. The growth stops as the substrate concentration in the second reactor diminishes.



**Figure 4.3** Model responses when

The results shown in Figure 4.4 are quite similar to the first simulation. A deeper decrease in is found (= 4.7 g COD m-3) when the value of is increased by 0.1 and the value of by 0.5. There is a slight increase in the level of biomass in the effluent (= 180 g COD m-3) and a recycle stream is considered in this case as is assigned as a positive value.



**Figure 4.4** Model responses when

Since the improvement in substrate removal was achieved by increasing both the values of , an investigation of the impact of varying a single parameter on substrate removal rate is carried out. is kept as an constant as 0.7 and a gradual increase in from 0.5 to 20 is suggested. As a result of the simulation, a tiny improvement in the substrate removal is achieved.

**4.4 Model Optimization**

In this section, the optimal design of this model based on the analytical method by Harmand et al (2003, 2004, and 2005) is initially presented. It demonstrates a pattern of how to systematically solve a nonlinear optimization problem. This example also provides valuable optimal solutions with which we can validate the ability of the dominating numerical and heuristic algorithms in Sentero and Copasi.

**4.4.1 Manual Optimization**

Adjusting design parameters intuitively to find the best parameter combinations in order to maximize model performance is found to be an inefficient method, as hundreds of simulations may be required as well as presenting plenty of simulation results (e.g. there are too many uncertainties in the simulation results shown in the above figures, as we are not sure whether the model with such parameter combinations meets the objective). Implementation mathematical optimization approaches on the model is thus carried out in section 4.4.3 as these methods (such as linear programming, nonlinear programming and mixed-integer nonlinear programming) take the advantages of the analytical properties of design problems to yield a sequence of points that converge to a global optimal solution.

**4.4.2 Model Optimization Using the Analytical Method**

The main objective of this minimal model is to yield the minimum total required reactor volume. The model is initially solved using the analytical method based on the gradient descent method. The optimization problem (Equation 4.2), expressed as a function of , and , is formulated by simplifying the expression of total volume by ignoring the constant terms, and , which have a minor effect on the determination of optimal solutions. The objective function is displayed as:

(4.2)

(Harmand et al., 2003, 2004 and 2005)

where: . , which is formed based on the Monod kinetics. Some physical considerations regarding the system yield the following constraints:

(4.3) (Harmand et al., 2003, 2004 and 2005)

The strategy for minimizing the objective function is divided into two phases. One can either minimize the function or the second term of the optimization expression. Firstly, is a continuous function on the closed interval of [0, ] and is differentiable on the open interval of (0, ). It is also calculated that the function of equals to 0 and **. According to the Rolle and Intermediate theorems (James et al., 2007), it can be concluded that this function is less than or equal to zero when it is at its minimum point , and also has two roots, namely, and .

Two different sets of optimal results for this model can be generated depending on the position of the two roots.

Case 1: when is on the interval of (), there is a unique set of optimal solutions leading to the minimum total volume, which includes =1, =0.

Case 2: when is on the interval of (), there exists an infinity of optima ( and ) that lie on the following equation. In addition, varies from 0 to 300 g COD m-3:

(4.4)

In contrast to Harmand’s work(2003, 2004 and 2005), we, here, quantify the solutions for the problem when case 2 is considered. It thus chooses a high specific value for , as 71.5 g COD m-3. The corresponding optimal results are summarized in Table 4.2. This is to investigate the impact of a high valued constraint () on the model performance, as well as the correlation between and .

**Table 4.2** Optimal model results when = 71.5 g COD m-3

Result

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Method |  |  | (m3) | (m3) | Objective  (m3) |
| Analytical method | 0.1 | 17.6 | 422.5 | 0.7 | 423.2 |
| 0.2 | 15.5 | 422.5 | 0.7 | 423.2 |
| 0.3 | 13.5 | 422.5 | 0.7 | 423.2 |
| 0.4 | 11.4 | 422.5 | 0.7 | 423.2 |
| 0.5 | 9.3 | 422.5 | 0.7 | 423.2 |
| 0.6 | 7.3 | 422.5 | 0.7 | 423.2 |
| 0.7 | 5.2 | 422.5 | 0.7 | 423.2 |
| 0.8 | 3.1 | 422.5 | 0.7 | 423.2 |
| 0.9 | 1 | 422.5 | 0.7 | 423.2 |

The calculation of the optimal values of is based on Equation 4.4 by keeping as a fixed value to achieve the optimal value of in a first order equation. By gradually increasing the value of by 0.1 in each computation, the corresponding value of can be calculated. The relationship between the input flow rate to the first reactor and the recycle flow rate is a monotonic decreasing trend. An increase in the input flow rate results in a decreased recycle flow rate. The size of the first reactor determined in each group is significantly greater than that of the second reactor. This thus leads to a larger hydraulic retention time for substrate degradation. The optimal model design for case 2 is illustrated in Figure 4.5.

, 

**Figure 4.5** Optimal model design for case 2

**4.4.3 Model Optimization Using the Numerical Method (PPT)**

Since the model was successfully structured and simulated in Sentero and Copasi, we decide to implement a numerical optimization method (the proximate parameter tuning algorithm, PPT) to find the optimal solutions for the model. This is also to validate the solutions given by the analytical technique.

Before implementing the PPT algorithm, a few operation options should be considered. For example, the target to be minimized is the sum of the total reactor volume; and , as the design variables, will be tuned; , as the constraints, should be chosen as a specific value in each run, otherwise the reactor volume will approximate to zero, which is not reasonable for biological systems. Finally, it is necessary to set number of iterations (as the PPT algorithm is an iterative technique that repeats the search until a good agreement between nominal values and real target features or maximum number of iterations is achieved). Usually, the higher the number of iterations, the better the model performance. The optimal solutions with different constraints are determined and displayed in Table 4.3.

**Table 4.3** Optimal results determined using the PPT algorithm when the constraint () is defined as specific low values

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Optimal result | Set 1 | Set 2 | Set 3 | Set 4 | Set 5 | Set 6 |
| (m3) | 527 | 572 | 619 | 725 | 1555 | 4182 |
| (m3) | 165 | 213 | 261 | 375 | 1197 | 3830 |
|  | 1 | 1 | 1 | 1 | 1 | 1 |
|  | 0 | 0 | 0 | 0 | 0 | 0 |
| (g COD m-3) | 5 | 3 | 2 | 1 | 0.1 | 0.01 |

There are 6 different sets of optimal results (each with a distinct constraint) shown in Table 4.3 when the algorithm is run with an iteration number of 2000 (this number could be less for a simple model). The PPT algorithm yields the same optimal values of parameters as those of the analytical method, as =1 and =0. It is thus observed that the required volume in this model is inversely proportional to the value of the constraint (). This can be understood from the process point of view that biomass requires a sufficiently large hydraulic retention time to absorb/degrade substrate when a strict discharge regulation is given. Figure 4.6 displays the optimal model design determined using the PPT algorithm when .

, 

**Figure 4.6** Optimal model design when

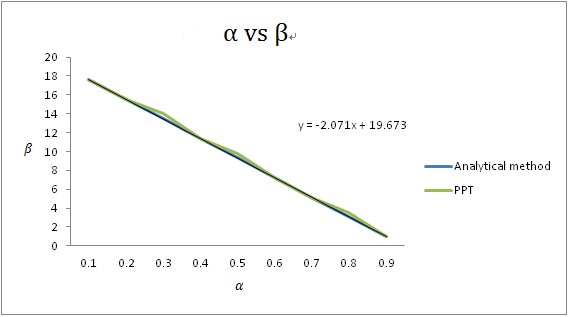
In Figure 4.6, all the fresh feed is fed to the first reactor in which the substrate is consumed at the highest rate. The size of the second reactor is relatively small. It is prepared to treat the substrate escaping from the first reactor due to the saturated biomass growth. The allocation of a recycle stream between two units is not required, as sufficient amounts of biomass in the first reactor are found and the concentration of substrate in the second reactor is maintained at a very low level.

Since a good agreement on the determined optimal results between the PPT algorithm and the analytical method (when a low value of the constraint *S*2 was considered) was achieved, validating the optimal results for the other case (when ) is also of interest. The strategy to achieve this consists of 9 runs in each of which the constraint is kept as a large value (e.g. 71.5 g COD m-3) as to be consistent with that in the analytical optimization. A gradual increase in the value of by 0.1 in each run is also suggested. The corresponding optimal solutions are shown in Table 4.4.

**Table 4.4** Optimal model results using the PPT algorithm when S2>>S1’

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Result  Method |  |  | (m3) | (m3) | Objective  (m3) | Constraint  (g COD m-3) |
| PPT | 0.1 | 17.6 | 422.5 | 0.7 | 423.2 | 71.5 |
| 0.2 | 15.5 | 422.5 | 0.7 | 423.2 | 71.5 |
| 0.3 | 14 | 422.5 | 0.7 | 423.2 | 71.5 |
| 0.4 | 11.4 | 422.5 | 0.7 | 423.2 | 71.5 |
| 0.5 | 9.8 | 422.5 | 0.7 | 423.2 | 71.5 |
| 0.6 | 7.3 | 422.5 | 0.7 | 423.2 | 71.5 |
| 0.7 | 5.2 | 422.5 | 0.7 | 423.2 | 71.5 |
| 0.8 | 3.5 | 422.5 | 0.7 | 423.2 | 71.5 |
| 0.9 | 1 | 422.5 | 0.7 | 423.2 | 71.5 |

Unsurprisingly, the PPT algorithm in this case performs similarly to the analytical method. There is a gradual decrease in the value of when the value of increases. In addition, the volume of the second reactor approximates to zero. A graphical comparison between the determined optimal solutions by the two methods is displayed in Figure 4.7.

****

**Figure 4.7** Optimal values of and when

The optimal values of parameters achieved by the PPT algorithm fit very well to those by the analytical method, apart from the tiny deviations at some points. The optimal value of  is inversely proportional to the value of  and when rises to 0.9, the values of  from both methods converge to one. These common features prove the robustness, validity and flexibility of the PPT algorithm. The optimal model design is illustrated in Figure 4.8.



**Figure 4.8** Optimal model design when

**4.5 Testing a Variety of Optimization Methods in Copasi**

Validating a range of numerical and heuristic optimization methods (such as: Levenberg-Marquardt, evolutionary programming, genetic algorithm, particle swarm and so on) in Copasi using this simple model is also carried out and discussed in this chapter. The algorithms with the best performance in terms of having a low CPU time and small sum of squared error of residuals (RSS) to target values will be selected and further applied to the more complex synthesis problems of wastewater treatment plants as discussed in chapter 6.

The simple model in Copasi with each algorithm is implemented 9 times, in each of which the iteration is set as 2000 (apart from simulated annealing and praxis) to ensure more reliable results attained and the value of is gradually increasing by 0.1 in each run, starting from 0.1 at the first run to 0.9 at the final. The performance of each algorithm is shown in Table 4.5.

**Table 4.5** Performance of each optimization method

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Optimization algorithm | Sum of squared error of residuals | CPU time (min) | Iteration | Run |
| Particle swarm | 0.65 | 37 | 2000 | 9 |
| Levenberg-Marquardt | 4107 | 0.2 | 2000 | 9 |
| Evolutionary programming | 1582.9 | 14 | 2000 | 9 |
| Genetic algorithm | 952.9 | 25.4 | 2000 | 9 |
| Random search | 53.9 | 0.8 | 2000 | 9 |
| Simulated annealing | 1455.8 | 68.5 | N/a | 9 |
| Praxis | 2565 | 1.5 | N/a | 9 |

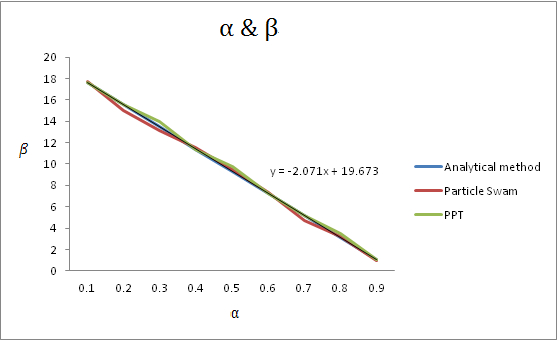
Having achieved high values of the sum of squared error of residuals to the target value, Levenberg-Marquardt, evolutionary programming, generic algorithm, simulated annealing and praxis do not fit the model and are eliminated from the list. Random search seems to be a choice as it provides smoother optimal solutions with a tolerable value of RSS. However, this method is only considered to be used for simple models as local minima would be searched in most cases. Particle swarm among all approaches generates the smallest RSS to the regression with a relatively low CPU time and is then considered as a robust and efficient algorithm to deal with nonlinear optimization problems. The optimal solutions determined using the particle swarm algorithm are summarized in Table 4.6.

**Table 4.6** Optimal results by particle swarm

Result

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Method |  |  | (m3) | (m3) | Objective  (m3) | Constraint  (g COD m-3) |
| Particle Swarm | 0.1 | 17.7 | 422.3 | 1 | 423.3 | 71.5 |
| 0.2 | 15 | 411.3 | 12 | 423.3 | 71.5 |
| 0.3 | 13.1 | 414 | 9.3 | 423.3 | 71.5 |
| 0.4 | 11.5 | 423.1 | 0.1 | 423.2 | 71.5 |
| 0.5 | 9.4 | 423.1 | 0.1 | 423.2 | 71.5 |
| 0.6 | 7.4 | 423.1 | 0.1 | 423.2 | 71.5 |
| 0.7 | 4.7 | 412.8 | 10.5 | 423.3 | 71.5 |
| 0.8 | 3.2 | 423.2 | 0.1 | 423.3 | 71.5 |
| 0.9 | 1 | 421.6 | 1.6 | 423.2 | 71.5 |

The total required reactor volume determined in each run in Table 4.6 approximates to 423.3 m3 with a constraint of = 71.5 g COD m-3. It is found that the determined optimal solutions () are very consistent with those by the analytical method. In addition, a graph assembling the optimal solutions achieved by the analytical method, the PPT algorithm and the particle swarm algorithm is displayed in Figure 4.9:



**Figure 4.9** Optimal values of and achieved by the analytical method, the PPT algorithm and the particle swarm

As can be seen, the results determined by the PPT algorithm and the particle swarm algorithm tightly fit those by the analytical method. An increase in the optimal value of leads to a decreased value of.

In conclusion, the growth of bacteria in the continuous reactors behaves in a nonlinear fashion with respect to the concentration of substrate as well as time. There is an exponential increase in the amount of biomass at the early stage of simulation and the growth stops until the substrate is depleted.

Implementing a variety of optimization algorithms on the model, two sets of optimal design with different constraints have been determined. The first optimal configuration consisting of two CSTRs in series with a single stream feeding to the first unit performs very well on the substrate removal. It is found that the size of reactor is inversely proportional to the concentration of substrate in the effluent. The feed in the other optimal configuration is distributed among the two reactors and a recirculation loop between the second reactor and the first one is suggested. In spite of achieving the minimum total required volume compared to the first design, a lower efficiency in substrate removal is determined.

The performance of each optimization approach has been also evaluated, in which the particle swarm algorithm generating the smallest sum of squared error of residues with less computational effort is selected to be used to deal with the highly nonlinear problems of wastewater treatment plants in chapter 6.

**4.6 Summary**

A minimal model of the activated sludge process describing organic carbon degradation was simulated in order to investigate the possible benefit of using a distributed feed system and a recycle stream as well as providing a basis for evaluating a range of optimization algorithms in Copasi. The key findings can be summarized as follows:

* The simulation results determined in section 4.3 show that the value of has the greatest impact on model output features as the concentration of substrate in the second reactor decreases significantly with an increasing value of . However, a tiny improvement in substrate removal is observed with an increasing value of . This is mainly attributed to the depletion of the substrate in the second reactor due to the high growth rate employed. In addition, only a small amount of substrate appears in the recycle stream.
* Two optimal design scenarios with different constraints are determined using the analytical method. One is that the process flowsheet consists of two CSTRs in series with a single stream feeding to the first reactor.A maximum substrate removal rate is achieved with the employment of sufficient large reactors. The other one demonstrates that the minimum total required reactor volume can be obtained with distributed feeds and a recirculation loop. However, this results in a poor performance in terms of substrate removal.
* Validating such optimal design solutions using a variety of optimization algorithms in Sentero and Copasi shows a good agreement on the determined optimal results between the analytical and numerical and heuristic optimization algorithms. Particle swarm, among all approaches, generating the smallest RSS to the regression with a relative low CPU time, is considered as a more robust and efficient one to deal with nonlinear programming problems. The continuing using of this method to solve more complex problems is discussed in chapter 6.

1. **A Case Study- Modelling of a WWTP in China Using BioWin**

**5.1 Preface**

In this chapter we demonstrate the diversity of optimization used in the field of wastewater treatment from another philosophical perspective. We use a commercial wastewater simulation package (BioWin) to model an industrial wastewater treatment plant. We further propose a physical retrofit, instead of using optimization methods, to improve the plant performance. Integrating the existing plant configuration with two anaerobic digesters not only demonstrates the potential for saving energy, but also reduces the impact of high COD loads to the plant while minimizing the sludge production.

**5.2 Modelling of the ZhouCun Wastewater Treatment Plant**

Water pollution, all over the world, has become one of the most critical problems that harms the environment and threatens human life. Due to the lack of advanced technologies or experience of running wastewater treatment plants, people in developing countries suffer from a shortage of drinking water. China is one of the typical cases, having plenty of existing wastewater treatment plants, only 10% of which can effectively produce clean effluents that satisfy discharge regulations (Chen et al., 2009). Most wastewater treatment plants are energy intensive units, especially for those dealing with wastewater under aerobic conditions as a considerable amount of oxygen is required to feed to the systems. To improve plant designs in order to achieve purified effluents while saving energy and money is a long-term task to fulfill.

The aim of this chapter is to improve the performance of an industrial wastewater treatment plant in China based on the use of modelling approaches. This task involves a steady state simulation based on the constant input and a dynamic simulation based on the consecutive inputs of 25 days provided by the plant. We introduce a physical retrofit (adding two anaerobic digestion models) to the validated steady state model to improve its performance. It is expected to offset a considerable amount of energy consumed due to the aeration by the generation of renewable gas (methane).

The ZhouCun wastewater treatment plant, the simulation target, is located at ZiBo city in northern China. The plant treats about 45000 m3 of sewage daily based on the technology of hydrolytic-acidification + A2O(Everbright Water, 2011). A2O (Anaerobic-Anoxic-Oxic) is one of the sophisticated biological methods evolved from the traditional activated sludge process. It can achieve a better performance for nitrogen and phosphorous removal. Requiring a lower hydraulic retention time and reducing operation costs make it more competitive to other biological treatment processes. Table 5.1 summarizes the information of the inlet wastewater to the plant and Table 5.2 displays the design parameters of the plant.

**Table 5.1** Average inlet wastewater compositions to the ZhouCun plant

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Inlet wastewater composition | COD  (g CODm-3） | BOD5  (g BODm-3） | Inorganic *SS*  (g SS m-3） | SNH4  (g N m-3） | TP  (g P m-3) |
|  | 254 | 93.11 | 386 | 27.44 | 10 |

**Table 5.2** Design parameters of the ZhouCun plant

|  |  |  |  |
| --- | --- | --- | --- |
| Design parameter | Anaerobic zone  () | Anoxic zone  () | Aerobic zone  () |
| Reactor volume  (m3) | 6000 | 23000 | 40000 |
| Total flow rate () to each zone  (m3 d-1) | 89075 | 89075 | 89075 |
| Hydraulic retention time HRT (h) | 1.6 | 6.2 | 10.8 |

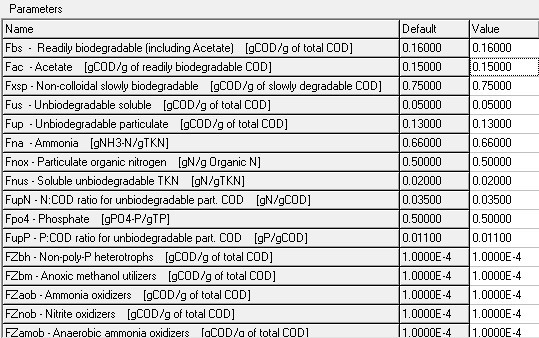
Due to the lack of modern instrument operated in the plant for the detailed analysis of incoming wastewater quality, we are here restricted to focus on the analysis of total COD, BOD5, and TSS in the effluent. According to the characteristics of the inlet wastewater compositions given in Table 5.1, it is concluded that the raw wastewater to the plant mainly originates from both industrial and municipal applications. COD and, as the major sources for biomass growth, are given as 254 g COD m-3 and 27.44 g N m-3 respectively. Three reactors are arranged in an order of the anaerobic reactor followed by the anoxic and by the aerobic, the volume of each is given as = 6000 m3, = 23000 m3 and = 40000 m3.

BioWin, as the dedicated commercial simulation tool, is used for modelling of the ZhouCun wastewater treatment plant. Providing an extended library of predefined process modular units, the model configuration in BioWin can be easily constructed by connecting the selected units. ASM3 is chosen as the biological model to describe the biological reactions taking place in the activated sludge process. The double exponential settling velocity function of Takács et al(1991) is selected to model the settling process in the settler.

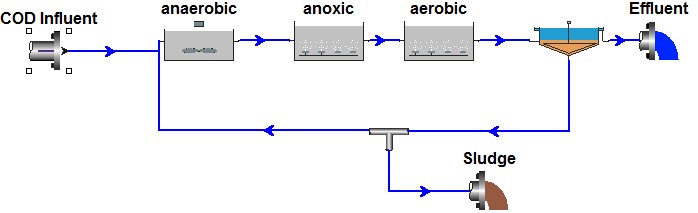
**5.2.1 Steady-State Model Simulation**

Steady-state models describe that anything involved in systems does not change with time. The purpose of designing such models is that the design specifications of most systems are associated with the steady-state characteristics. In another word, steady-state solutions often reveal a fairly amount of information regarding the general model structure, robustness and validity. In addition, steady-state model simulation is an indispensable step prior to dynamic simulation. The latter simulation aims to investigate the impact of dynamic inputs on process performance.

Due to the lack of detailed inlet COD compositions, we decide to employ the default COD fraction value (shown in Figure 5.1) proved by the BioWin influent module. The total inlet flow rate to the model is 46063 m3 d-1 and the flowsheet of A2O model in BioWin is displayed in Figure 5.2.



**Figure 5.1** Inlet wastewater fractions proved by BioWin influent module



**Figure 5.2** A2O model configuration

The A2O configuration consists of three reactors in series, namely: anaerobic, anoxic and aerobic. The raw wastewater with the mixed liquor suspended solids (containing biomass and oxidized material) from the sedimentation tank is primarily fed to the anaerobic reactor in which phosphorous is released as soluble phosphates. Meanwhile, the reaction of ammonification takes place where soluble organic nitrogen is converted to free and saline ammonia by the active heterotrophs. The effluent leaving the anaerobic unit is conveyed to the anoxic reactor where nitrate is biologically reduced to nitrogen gas. The consumption of organic matter at this stage provides all the energy required for denitrification. The aerobic reactor is the final biological phase where large quantities of organic matter, nitrogen and phosphorus are taken up due to the growth of facultative bacteria and the corresponding products are further fed to the secondary clarifier in order to separate clean effluent from mixed liquor suspended solids. Some portion of the sludge in the clarifier is again recycled back to the influent and the rest is treated as waste sludge. The inlet flow rate () to the system is given as 46063 m3 d-1 and the recycle flow rate is 43012 m3 d-1.The hydraulic retention time (the length of period the biomass remains in units) for each reactor is thus calculated as: 1.6h, 6.2h and 10.8h respectively. The simulation results of the steady state model are summarized in Table 5.3.

**Table 5.3** Model simulation results

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Parameter | Inlet wastewater parameter | Plant output feature | Simulation result with default inlet fractions | Simulation result with adjusted inlet fractions |
| Total inlet flow (m3 d-1) | 46063 | 46063 | 46063 | 46063 |
| Total COD g COD m-3 | 254 | 51.18 | 64.6 | 52.2 |
| Total Nitrogen  (g N m-3) | 41.58 | 19.35 | 21.16 | 19.63 |
| Total P  (g P m-3) | 10 | 2.47 | 5.28 | 5.27 |
| Nitrate  (g N m-3) | 0 | - | 11.75 | 13.59 |
| HRT (h) | - | 18 | 18.6 | 18.6 |
| SRT (d) | - | 19.26 | 19.35 | 19.35 |
| Recycle rate | - | 0.93 | 0.93 | 0.93 |
| (g SS m-3) | - | 6.36 | 5.5 | 5.6 |
| Total BOD  (g BOD m-3) | 93.11 | 4.61 | 34.99 | 4.01 |
| (g N m-3) | 27.443 | 1.49 | 1.57 | 1.41 |
| Air flow rate to the aerobic (m3 h-1) | - | 3600 | 3600 | 3600 |

There is a good verification between the model simulation results with the default inlet factions and the plant output features as the concentrations of COD and in the effluent in the model are significantly reduced from 254 g COD m-3 and 41.58 g N m-3 to 54.6 g COD m-3 and 21.16 g N m-3 respectively. However, a 10% higher in COD,ef in the simulation results compared with the real target value is insufficient to prove a good validation.

The analysis of that 10% higher in COD,ef is attributed to a little disagreement in the inlet COD composition distribution between the BioWin influent modular unit and ASM3. Acetate does not appear as an individual to be involved in any reactions in ASM3. Such a component exists in the form of the readily biodegradable COD which is directly consumed for biomass growth. However, BioWin COD influent module separates acetate from readily biodegradable COD and assigns it a default fraction of 0.15 of total inlet COD. This thus results in an additional fraction of untreated COD in our model simulation. An increase in the fraction of non-biodegradable COD compared to that of BioWin influent module should also be considered, as the actual incoming wastewater to the model originates from both industrial and municipal applications. The fractions of *Fus* (non-biodegradable soluble COD) and *Fup* (non-biodegradable particulate COD) are increased from 0.05 and 0.13 to 0.17 and 0.2 respectively. It also assumes that there is some biomass in the inlet wastewater feeding to our model, which accounts for 7.4% of the total COD.

The simulation results shown in the last column of Table 5.3 are obtained from making few modifications to the default fractions using the steady state solver provided by BioWin. It is noted that a good model validation is achieved as the concentrations of COD and nitrogen in the model are very close to those from the plant, apart from the phosphorous aspect which is not taken into account in this study. The CPU time required to solve the steady state model is about 9 seconds and an Intel Core i-3 of 2.4 GHz with 4GB of RAM is used.

**5.2.2 Dynamic-State Model Simulation**

Wastewater treatment processes are inherently dynamic because of having varying flow and loads. Time, as a major parameter, is considered in the process of this kind. The development of a dynamic model of wastewater treatment plant under a computational circumstance is of necessity as it can help predict the performance of time-dependent systems in practice. With given a consecutive influent data of 25 days from the plant, a dynamic model is simulated. The simulation results are displayed in the following figures:

**Figure 5.3** Simulation result - COD,ef

**Figure 5.4** Simulation result -

**Figure 5.5** Simulation result - TSS,ef

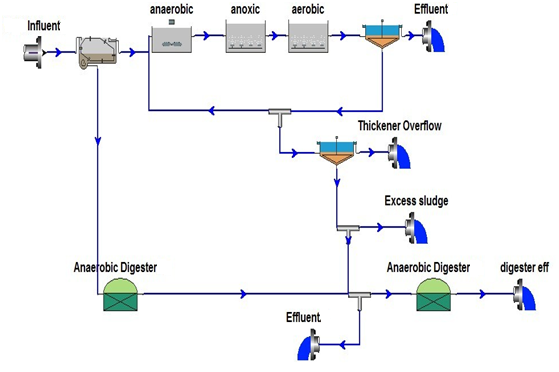
According to the above figures, a good agreement between the model and the plant in terms of the concentrations of COD,ef and is achieved, despite that there is a small flaw in the profile that a sample from the plant reaches a peak of 8.5 g N m-3 which is significantly higher than both the averaged simulation result and the discharge limit. Such a peak may be caused by two reasons (for example, 1. the sudden increase in loading rate on that day or 2. the failure in the operation to the aerobic tank). Figure 5.5 illustrates a large deviation in the concentration of total suspended solids between the model and the plant. A smoother trend of the total suspended solids is achieved in the model. A longer CPU time (35 seconds) is required to solve the dynamic model taking into account the course of 25 days as compared to the steady state model.

**5.3 Model Retrofit**

Like most aerobic-based wastewater treatment plants, the ZhouCun plant is also confronted with the excessive consumption of energy due to aeration. They have made a few attempts to save energy through using different control strategies or adjusting operating parameters but with a little improvement in return. Two options here are available that can potentially improve the plant performance:

* To integrate the well-established renewable options with wastewater treatment plants in order to offset the energy consumed during the operation. For example, using the biogas (methane) from anaerobic digestion processes.
* To improve the efficiency in water reuse by consumers and in energy used by water industrial applications.

From the process synthesis perspective, option 1 is more suitable to be applied to our model. The allocation of anaerobic digestion models to the existing configuration can generate large amounts of biogas (methane) that can offset a great deal of energy consumed during the operation. Apart from this, producing 90% less of sludge compared to the activated sludge process and adapting high COD loads ranging from 20-35 kg COD per m3 per day are the other two attractive aspects that make this retrofit possible. The modified model flowsheet is displayed in Figure 5.6.



**Figure 5.6** Modified model flowsheet-A2O+anaerobic digestion model (ADM)

Apart from adding two anaerobic digesters to the flowsheet in Figure 5.6, the allocation of a primary sedimentation tank is also considered as it is to accumulate the incoming COD into the dense suspended solids that are required by the anaerobic process. It can be seen that the sludge from the primary and the secondary settling tanks after the dewatering is conveyed to the secondary anaerobic digester model allocated at the tail end of the A2O configuration. The performance of the anaerobic digesters is summarized in Table 5.4

**Table 5.4** The performance of the anaerobic digesters

|  |  |  |
| --- | --- | --- |
| Parameter | Value | Unit |
| Methane content | 570.9 | m3 d-1 |
| Volatile suspended solid | 20.4 | kg SS m-3 |
| Total suspended solid | 106.88 | kg SS m-3 |
| Total COD | 32.3 | kg COD m-3 |
|  | 0.73 | kg N m-3 |
| HRT | 10 | d |
| pH | 7 | Na |

With given appropriate design and operating parameters, the model achieves a production of methane of 570.9 m3 d-1 at 350C when it is simulated at a steady state condition. The concentrations of total COD and in the effluent are estimated as 32.3 kg COD m-3 and 0.73 kg N m-3 respectively. Due to the accumulation of solids in the reactors, the concentration of the total suspended solids is determined as 106.88 kg SS m-3. The CPU time required to solve the retrofit model is 19 seconds. The detailed calculations of energy recovery due to the energy released from the generated methane are below shown:

* Gas flow generated = 875 m3 d-1
* Methane content = 570.9 m3 d-1 (as 65.24% of overall gas)
* Methane density = 0.7 kg m-3
* The total mass of methane is 0.7\*570.9 = 400 kg d-1

According to Guisasola et al (2008), the release of 1kg of methane is roughly equivalent to the generation of 20 kWh of electricity

* The power recovered due to the methane production in the anaerobic digesters per day is: 400\*20 = 8000 kWh d-1
* The power consumption of per liter of liquid in the plant = 0.277kwh m-3
* The total inlet flow rate is 46063 m3 d-1
* The total power consumption in the plant is 46063\*0.277 = 12759.5 kwh d-1.
* The net power consumed = the total power consumption – the power recovered due to the generated methane = 4759.5 kwh d-1.

Approximately, 8000 kWh power is recovered daily due to the running of two anaerobic digestion reactors. The total power consumption on the plant is thus cut by 2/3. Adding physical retrofits to existing industrial plants is an alternative approach that can complement the defects of original processes and improve plant performance.

However, this attempt is not yet a complete and mature process synthesis approach as some essential design aspects (such as the investment and operating costs of the added equipment) are not taken into consideration. This, at the moment, only delivers an optimization idea from different process perspective.

A more systematic optimal design of industrial plants is carried out in chapter 6. We focus on the use of optimization approaches to determine optimal process configurations for plants while evaluating overall costs for plants. In addition, we investigate the possible benefit of the optimal design of dynamic wastewater treatment plants subject to time-varying inputs.

**5.4 Summary**

In this chapter, we have demonstrated the use of a commercial wastewater simulation package (BioWin) to model an industrial wastewater treatment plant (the ZhunCun Plant) and further improved the plant performance by retrofitting the existing model configuration.

Coupling the two anaerobic digestion reactors with the A2O configuration of the ZhunCun plant achieves a production of methane of 570.9 m3 d-1. Converting to power, 8000 kWh of power can be recovered daily, which is approximately 2/3 of the total power consumption on the plant ever day. In addition, using the predefined settler model provided in BioWin more accurate plant performance in terms of effluent compositions at the steady state condition is obtained (e.g.).

Apart from energy recovery, there is a dramatic reduction in the sludge production in this retrofit design as the generated suspended solids are pumped to the anaerobic digestion reactors in which the complex organic matter can be easily degraded and 90% less of sludge is produced as compared to the activated sludge process.

1. **Optimal Design of Industrial Wastewater Treatment Plants (WWTPs)**

**6.1 Preface**

In this chapter, we present the systematic optimization of the process structure and the operating conditions of wastewater treatment plants based on ASM3. The objective is to minimize the total plant costs while complying with the effluent discharge standards. The novel contribution of this work is to take into account the dynamic variations in both feed compositions and flow rate as a part of model optimization. We further investigate the possible benefit of the dynamic design as compared to that under the steady state condition (i.e. using averaged inputs). This chapter is, therefore, divided into two parts: 1. steady state optimization of wastewater treatment plants and 2. optimal design of wastewater treatment plants subject to time-varying inputs.

First, to validate our optimization methodology for activated sludge plants we replicate building a published model of Alasino (2007) which is given in Figure 6.1. This task involves the comparisons of effluent quality and total plant costs between the two models. Implementing the particle swarm algorithm on the replicated model, it results in an optimal design providing an even lower total plant cost as compared to that determined by Alasino using the general algebraic modelling system (GAMS).

Modelling of an industrial wastewater treatment plant based on the methodology is afterwards developed. The systematic optimization of the model subject to averaged inputs (steady state) and time-varying inputs is carried out respectively and is discussed in part II. A further comparison between the results determined in these two scenarios will eventually yield a more robust and effective design.

**Part : Steady State Heuristic Optimization of WWTPs**

Due to the importance of the activated sludge process for carbonaceous and nitrogen removal and ease of manipulation, the market for the activated sludge process in developing countries has grown strikingly fast during the last few decades. As a result of dealing with massive amounts of sewage due to their economic and industrial expansion, a great many of treatment plants based on the prior design knowledge or trial-and-error pilot plants have been constructed. However, the expenditure on these plants has become a long-term issue.

Engineers/designers aim to improve the design of existing plants and strive to enhance the operation of equipment once it is installed. This, alternatively, is to achieve the largest production, the greatest profit, the minimum cost and so on. In most well-attended wastewater treatment plants the common objective is to minimize the total plant cost which is the sum of investment and operating costs. Mathematical modelling, as an alternative approach, has very significant advantages over traditional approaches in wastewater treatment engineering. It can facilitate the saving of time and money, minimizing risk due to operation as well as getting insight into process performance and has been widely used in many studies to facilitate the understanding of wastewater treatment process in both static and dynamic systems. The potential of this approach combined with powerful optimization has yet to be exploited to solve practical challenges in wastewater treatment plants.

**6.2 Methodology Validation with Alasino’s Model**

Validating our methodology for complex wastewater treatment plants is achieved by replicating the historic model determined by Alasino (Figure 6.1). A complete activated sludge plant model should consist of activated sludge model, hydraulic model and oxygen transfer model so that the real dynamic behaviour of plant can be described. The model configuration in Figure 6.1 consists of three aerobic reactors in series and a settlement tank.

=18309 m3 d-1

Settler

=8086 m3 d-1

=10360 m3 d-1

6099 m3

= 27 d-1

9096 m3

d-1

1083 m3

8 d-1

==11840 m3 d-1

=137 m3 d-1

**Figure 6.1** Configuration of Alasino’s model

The volume of each reactor in Figure 6.1 is given as , and with different allocated oxygen transfer coefficients as = 218, and . In contrast to Alasino’s model, an assumption here is made that there is a perfect separation for the mixed liquor suspended solids during the settling stage, thus the effluent stream should only contain soluble components. The design of settler model is, therefore, negligible so long as an appropriate mass balance equation for the sludge at the tail end of the process is considered. This assumption is discussed in more details in the following section. The total inlet flow rate () is given as 18446 m3 d-1, which has been distributed into two streams. One is feeding to the first reactor with a flow rate of 10360 m3 d-1 (is the coefficient of the total inlet flow rate varying from 0-1 and in this case is chosen as 0.56 ). , the remaining part of the total flow rate, feeds to the second reactor with a flow rate of 8086 m3 d-1. A recirculation stream () is linked between the ‘nominal settler’ and the first reactor. The recirculation flow rate is calculated by the product of and ( is the recycle ratio). The effluent flow rate () is given as 18309 m3 d-1 and the sludge flow rate () is estimated as 137 m3 d-1. The inlet wastewater compositions to the plant given in Table 6.1 are mainly divided into two categories, soluble (indicated by ) and particulate (indicated by). In addition, to aid the validation we compare and contrast the features of Alasino’s and our methodologies and the detailed information is displayed in Table 6.2.

**Table 6.1** Inlet wastewater compositions

|  |  |  |
| --- | --- | --- |
| Component | Concentration | Unit |
|  | 30 | g COD m-3 |
|  | 69.5 | g COD m-3 |
|  | 51.2 | g COD m-3 |
|  | 202.32 | g COD m-3 |
|  | 28.17 | g COD m-3 |
|  | 0 | g COD m-3 |
|  | 0 | g COD m-3 |
|  | 215.493 | g SS m-3 |
|  | 0 | g O2 m-3 |
|  | 0 | g N m-3 |
|  | 0 | g N m-3 |
|  | 36.425 | g N m-3 |
|  | 7 | g COD m-3 |
|  | 3.79 | n/a |

**Table 6.2** Comparison of features between Alasino’s and our models

|  |  |
| --- | --- |
| Alasino’s model | Our model |
| Clarifier modelled explicitly | Implicit clarifier modelling assuming perfect separation |
| Detailed economic cost functions | Detailed economic cost functions |
| Detailed modelling of activated sludge reactions | Detailed modelling of activated sludge reactions |
| Limited to steady state | Considers both constant and dynamic loadings (the latter of which is discussed in Part ) |
| Nonlinear algebraic equations (highly constrained) | Ordinary differential equations (less constrained) |
| Mathematical programming (MINLP) | Heuristic method- Particle Swarm |

Our approach has the important advantage of achieving an optimal plant design subject to time-varying inputs (dynamic state) whereas Alasino’s method is limited to the steady state design. Alasino uses the nonlinear algebraic equations to solve the model. However, we integrate the differential equations that comprise our model and it is rather un-constrained except for the simple bounds on some design variables. This is a relative easier task for the heuristic algorithm to complete a search for optimal solutions. In our modelling approach, we assume a perfect separation for treated effluent and do not explicitly design a sedimentation tank. A better separation can be achieved in Alasino’s model because of the placement of a settler model.

**6.2.1 Economic Modelling**

Apart from evaluating the effluent compositions, the estimation of total plant cost including investment and operating costs is another important aspect for assessing plant performance. Designers should make a trade-off between cost and effluent quality when designing an appropriate plant. The total plant cost can be defined as Net Present Value (NPV) and expressed as follows:

where: is the total investment cost and is the total operating cost. It should be noted that NPV is a slight misnomer (here we are following the notation of Alasino) since it is actually the Net Project Cost which we want to minimize rather than a Net Project Value which tends to imply a function to be maximized.

The total investment cost for activated sludge plants is the sum of the costs for tank construction, aeration systems, influent pumping station, sedimentation tank and sludge recirculation. The investment cost of the plants is expressed as follows:

where: is the investment cost for cost component for unit is the number of investment cost components. Since investment costs are incurred at the beginning of a project, this expression is suitable for both steady state and dynamic models. The detailed information of each investment cost component is summarized in Table 6.3.

**Table 6.3** Investment cost components

|  |  |  |
| --- | --- | --- |
| Component | Cost function | Parameter |
| Tanks |  |  |
| Aeration systems |  |  |
| Influent pumping station +screening |  |  |
| Sludge recirculation |  |  |

(Wright and Woods, 1993; Fels et al., 1997)

Modelling of the total operating cost () involves the consideration of the operating cost occurring in the future (e.g. over a plant life span of 20 years). (Equation 6.3) is the update term to calculate the future cost to the present value. The total operating cost for activated sludge plants includes the costs for aeration energy demand, pumping energy demand, effluent quality index, waste sludge disposal and external carbon source dosage rate. The expression of the operating cost for the plants is given as follows

where: is the annual operating cost for cost component . is the number of operating cost components. is the update term that calculates the future operating cost to the present value over the plant lifetime, is the interest rate, is the life span of WWTPs (a life span of 20 years will be generally considered in the following sections for calculating total plant cost).

In fact, Equation 6.2 is merely suitable for steady state models since the operating variables are time invariant and constant over the lifetime of plants. For dynamic models, there is a slight difference in the operating cost function in which the plant variables are time varying rather than constant. A daily operating cost calculated from the model outputs at the end of each day is considered and the total operating cost for dynamic models can be formulated as:

where: is the daily operating cost for cost component over day . The cost functions for operating components are summarized in Table 6.4.

**Table 6.4a** Operating cost components for the steady state case

|  |  |  |
| --- | --- | --- |
| Component | Function | Parameter |
| Aeration power |  |  |
| Pumping power |  |  |
| Effluent taxes |  | and |
| Sludge disposal |  | Excess sludge TSS |
| External carbon source dosage |  | Carbon consumption |

(Gillot et al., 1999)

**Table 6.4b** Operating cost components for the dynamic case

|  |  |  |
| --- | --- | --- |
| Component | Function | Parameter |
| Aeration power |  |  |
| Pumping power |  |  |
| Effluent taxes |  | and |
| Sludge disposal |  | Excess sludge TSS |
| External carbon source dosage |  | Carbon consumption |

(Gillot et al., 1999)

where: are the steady state costs in Table 6.4a and are replaced by their dynamic counterparts: in Table 6.4b (note that only are truly time varying since the other cost expressions do not contain time varying variables, however, we retain a general notation to conform to dynamic objective function. in Table 6.4a are the constant flow rates (m3 d-1) of internal recycle, external recycle and waste sludge. in Table 6.4b are the daily (time varying) flow rates (m3 d-1) of internal recycle, external recycle and waste sludge in the dynamic model. In addition, in either case is zero since there is no need to have an internal recycle stream in this treatment process configuration. is the volumetric liquid mass transfer flow rate(d-1). Note that is a constant parameter and so is the same for the steady state and dynamic cases. in Table 6.4a are the steady state concentrations of suspended solids, organic carbon and total nitrogen material in the effluent. in Table 6.4b are the daily (time varying) concentrations of suspended solids, organic carbon and total nitrogen material in the effluent.

* + 1. **Model Performance Comparison with Alasino’s model**

**6.2.2.1 Effluent Quality Comparison**

The effluent of our model is assumed to be completely clarified – i.e. only including soluble components which are , , and . The model achieves 99.4 % removal rate for and 99.9% for the readily biodegradable COD and the corresponding concentration of is determined as 0.033 g COD m-3 and as 0.22 g N m-3. There is a considerable agreement between Alasino’s (98.4% for and 99.9% for readily biodegradable COD ) and our model results, as both have significantly reduced the level of COD and in the system. However, a perfect match between each component is not determined and the comparison related to the solid components between two models is not feasible because our model has a perfect separation in this simulation flowsheet, whereas Alasino, who uses a model of the secondary clarifier, does not.

However, there is a major disagreement when comparing the effluent nitrate between two models which, we believe, highlights an important error in Alasino’s model. The concentration of total nitrogen in the effluent in Alasino’s model was determined as 2.18 g N m-3 which is an order of magnitude lower compared to our value of 27 g N m-3. This latter value better matches the total nitrogen entering the system. In addition, being operated under aerobic conditions for all three units, there is no possibility for the biomass to denitrify the high-yielded nitrite even assigning relatively lower values of for the last two reactors. In summary, therefore, we consider our model response, with the concentration of total nitrogen of 27 g N m-3 in the effluent, truly reflects the real behaviour of the aerobic treatment process when dealing with nitrogen removal despite the fact that this far exceeds the results given by Alasino. The effluent quality comparison between two models is summarized in the following table.

**Table 6.5** Effluent compositions of two models

|  |  |  |
| --- | --- | --- |
| Effluent compositions | Alasino’s model | Our model |
| (g COD m-3) | 0.1 | 0.1 |
| (g N m-3) | 0.69 | 0.22 |
| (g N m-3) | 2.18 | 27 |

**6.2.2.2 Economic Comparison**

It is also of interest to compare the expenditure on both models since they have achieved a good consistency between their process outcomes. As was mentioned previously, total plant cost is the sum of operating and investment costs. Obviously, the investment costs are fixed due to the nature of design, whereas the operating costs vary since their cost functions depend on both design parameters and continuous variables. For example, the cost for sludge disposal is associated with flow rate and the concentration of total suspended solids, the latter of which is a dependent variable on some design parameters, especially on SRT.

With given a design plant life span of 20 years and a 5% interest/discount rate, the comparison of the operating costs between two models is displayed in Figure 6.2.

**Figure 6.2** Operating costs of two models

First of all, the cost for the external carbon dosage is considered to be zero. This is attributed to the type of the process which has all three reactors in series operated under aerobic conditions. Generally, the organic carbon source in raw wastewater feeding to the activated sludge process plants is sufficient for the biomass growth due to COD degradation and nitrification. Only the process that triggers denitrification under anoxic conditions may have a special requirement on a higher ratio of COD/TKN. The total cost for pumping energy demand is computed as €149300, which is proportional to the flow rates of the recycle and the waste streams. Energy consumed due to the aeration has been a long-term issue in practice, as it accounts for the major fraction of the total power consumption during treatment. As all three reactors are operated under aerobic conditions, the operating cost for aeration energy demand in this case is inevitably high at €945800. Treatment of wasted sludge is also a complicated process which is further separated into processes, such as: dewatering, thickening and so on. The spending on sludge production and disposal is calculated as €1460000, which accounts for half of the total operating cost. Actually, the rate of sludge produced depends very much on the concentration of suspended solids which is directly controlled by SRT. A longer SRT leads to a high concentration of sludge thus resulting in a high cost for sludge disposal. In comparison with Alasino’s model, it has achieved similar cost on each operating sector, apart from the aeration energy, which is estimated as only half of that by Alasino. We consider that this is another error occurred in Alasino’s model. Turning our attention to investment costs, Figure 6.3 illustrates the investment cost breakdown for the two models.

**Figure 6.3** Investment costs of two models

The estimation of total investment cost for our model includes the consideration of the costs for different process units. It can be seen that the costs in our model are identical to Alasino’s, except for the settler which is not explicitly modelled in our simulation flowsheet.

The total expenditure on sludge pumping related to the recycle flow rate is calculated as €149300. The cost for aeration device based on its characteristic dimension (the oxygen capacity) is determined as €171000. The influent pumping station considers the costs related to concrete, screws and screening, and its characteristic dimension is the influent wastewater flow rate. The overall cost for pumping station is estimated as €269000. The expenditure on tank construction is the largest slice of the total investment cost, accounting for 78.7%, as €1740000. The cost of each aspect of two models is summarized in the following table:

**Table 6.6** Total costs of two models

|  |  |  |
| --- | --- | --- |
| Cost | Alasino’s model | Our model |
| * Operating cost (over a plant life span of 20 years) | | |
| Pumping energy | €149300 | €149300 |
| Aeration energy | €1844000 | €945800 |
| Sludge disposal | €1411000 | €1460000 |
| * Investment cost | | |
| Tank construction | €1740000 | €1740000 |
| Aeration system | €171000 | €171000 |
| Settler | €443000 | Na |
| Pumping station | €269000 | €269000 |
| Sludge recycle system | €33200 | €33100 |
| * Overall expenditure | | |
| Total plant cost | €6060500 | €4768200 |

**6.2.3 The Effect of Solid Retention Time (SRT) on Suspended Solids**

SRT is an important design and operating parameter to consider when designing wastewater treatment plants. It defines the length of time, on average, that the activated sludge remains in systems. It has been proved that the variation of SRT has a minor effect on soluble substrates removal when it is chosen as an appropriate value (El-Shorbagy et al., 2011). However, it is tightly bound to the estimation of sludge production as well as the concentration of solid components. This, therefore, significantly affects plant performance in terms of operating cost when a certain amount of sludge is wasted since sludge disposal is one of the major contributors to plant running costs. The characteristics of SRT can be visually defined in Figure 6.4 and Equations 6.5.

Mass balance equation:

(6.5)

Where: XR is the concentration of solid in the recycle, X3 is the concentration of solid in reactor 3.

(XR)

Settler

**Figure 6.4** Mass balance for suspended solids at the tail end of the simulation flowsheet

According to Equations 6.5, the amount of sludge leaving the third and final reactor is the sum of sludge being recycled and wasted. A high value of SRT operated in the system would lead to a rapid rise in the production of suspended solids due to the accumulated biomass in reactors. This thus increases the cost for sludge disposal.

**6.2.4 Model Optimization (Deterministic vs. Heuristic Optimization)**

The optimization problem of the model to be solved is to find the minimum total plant cost for the design given in Figure 6.1. In spite of this configuration having already been demonstrated as the lowest cost solution found by Alasino using a general algebraic modelling system (GAMS), we will introduce and apply an alternative optimization approach (the particle swarm) to the model and use the predetermined optimal solution as a starting point for the investigation of further optimized candidates. Given that it is not possible to guarantee global optimality for these problems, it is possible that our optimization terminates at an inferior point to that by Alasino, or, alternatively, is able to find better solutions for the model. The objective function to be minimized of this steady state model is the total plant cost which is the sum of the investment (Equation 6.1) and operating costs (Equation 6.2). It is expressed as follows:

**6.2.4.1 Advantages of Heuristic Optimization**

The highly combinatorial and nonlinear nature of the synthesis problems discussed in this work mean that they are on the limit of tractability for mathematical programming techniques such as that employed by Alasino using an MINLP formulation. The complexity increases still further if, as in the novel contribution of this work, the dynamic process behaviour is considered rather than just a steady state model based on averaged plant inputs. Given these considerations, even the tractability (never mind the optimality) of mathematical programming approaches is under question. It can therefore be beneficial to apply heuristic optimization algorithms in order to obtain good or near optimal process designs.

The ability of heuristic approaches to generate reasonable solutions in relatively short computational times can be attributed to the global search methods they use for the improvement of solutions. They tend to work well for problems that are not highly constrained and this, interestingly, is another benefit of our dynamic approach as opposed to the steady state approach of Alasino. Although the latter approach gives rise to problems of much lower dimensionality (due to the elimination of time), it does this at the expense of introducing a large number of nonlinear equality constraints that must be respected to ensure a feasible steady state solution.

Our approach, on the other hand, is based on integrating the differential equations that comprise the model and is therefore rather un-constrained except for the simple bounds on the design variables given in Inequalities 6.7. It is therefore an easier task for a heuristic optimization algorithm, such as particle swarm, to move around the largely feasible parameter space searching for improved solutions.

The broad popularity of heuristic algorithms arises from their relative ease of implementation and the fact that they can offer better over deterministic methods for solving certain types of complicated optimization problems. Although they have been shown to generate high quality solutions to a wide range of different problems, they cannot pretend to produce the exact solution in every case with certainty (Gilli, 2004). This, caveat, also applies local deterministic methods such as that employed by Alasino.

Since the optimal solutions by Alasino were determined by using mathematical programming techniques in the form of MINLP, there is the same uncertainty as to whether these steady state solutions are local or global optima. In this part of our research, our strategy is to use a dynamic model and apply stochastic search techniques in the form of particle swarm. The starting point for our search is the model configuration given by Alasino and the aim is to obtain possibly better solutions.

**6.2.4.2 Optimization Results**

Assigning lower and upper bounds onto the design parameters which are adjusted in the algorithm, defines a feasible region that includes all possible optimal solutions for the optimization problem. These constrained parameters are shown as follows:

(6.7)

where: is the upper bound for each of three reactor compartments; it is set as a large value as 10000 m3 that ensures a sufficient hydraulic retention time. A compartment will be eliminated from the model structure when it reaches its lowest bound at 0. A uniform value of for these three reactors is chosen as 10 h-1or 240 d-1. A compartment is defined as the anoxic reactor when is set as 0. The fractional parameter is in a range of 0-1 and, if it reaches its lower or upper bound, there will exist a single stream feeding to either of the first two reactors. The parameter is an arbitrary positive value having an upper bound of 30 which is the ratio between the rate of recycle and the flow rate into and out the plant. This parameter is related to the SRT and the upper bound of 30 days gives a high enough SRT for biomass to degrade most types of micro-pollutants in the activated sludge process. Generally, such a higher SRT is usually adapted in anaerobic processes due to the slow-growth rate bacteria. Any sludge-based treatment processes operated with a very short SRT will fail. For well mixed systems with no clarification, for example, SRT is equal to HRT – the hydraulic residence time. These will fail as there is no time for bacteria to grow in reactors before they have been washed out.

To comply with the discharge permitted limits, constraints of the dependent variables are also suggested and shown as follows:

(6.8)

A strict constraint on effluent quality can avoid activating the penalty for the discharge of high concentration of contaminants. This, however, results in an increase in biomass production and the requirement of high values of and further leads to a significant increase in the operating costs.

The particle swarm algorithm is implemented with an iteration number of 100 and a swarm size of 50. The corresponding optimal solutions are summarized in Table 6.7 and the optimal process flowsheet is displayed in Figure 6.5.

**Table 6.7** Optimal solutions

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Parameter | Optimal value | Starting value | Lower bound | Upper bound |
| (m3) | 8718 | 10000 | 0 | 10000 |
| (m3) | 5684 | 10000 | 0 | 10000 |
| (m3) | 2145 | 10000 | 0 | 10000 |
| (d-1) | 0 | 200 | 0 | 200 |
| (d-1) | 54.24 | 200 | 0 | 200 |
| (d-1) | 107.4 | 200 | 0 | 200 |
|  | 1 | 1 | 0 | 1 |
|  | 4 | 30 | 0 | 30 |
| SRT (d) | 3.97 | 30 | 0 | 30 |

18446 m3 d-1

8718 m3

Anoxic

5684 m3

Aerobic

2145 m3

Aerobic

73784 m3 d-1

18309 m3 d-1

*S*s=0.055 g m-3

*S*NH4=1.5 g m-3

*S*NO3=8 g m-3

137 m3 d-1

**Figure 6.5** Optimal design of our model

The new optimal process configuration determined consists of three biological reactors in series: an anoxic reactor followed by two aerobic reactors. The volumes of these three units are given as 8718 m3, 5684 m3 and 2145 m3 respectively. The value of in the last reactor is given as 107.4 d-1 which is double the value in the second reactor (54.4 d-1). All the feed is conveyed to the first reactor through a single stream with a flow rate of 18446 m3 d-1. The recycle flow rate is quadruple compared to that of Alasino’s model. Such a large recycle ratio implies that there is an excessive production of biomass and nitrate in the last reactor and to recycle the excessive nitrate to the anoxic reactor for denitrification (convert nitrate to nitrogen gas) is of necessity. As a result of denitrification, the concentration of nitrate in the effluent is controlled and estimated as 8 g N m-3. It is also found that the concentrations of readily biodegradable COD and in the effluent are determined as 0.6 g COD m-3 and 1.5 g N m-3 respectively. Figures 6.6 & 6.7 below show the comparison of the total plant cost between three models (Alasino’s model, the validated model and the optimized model using the particle swarm algorithm).

**Figure 6.6** Operating costs of three models

The total operating cost of our optimized model is estimated as €2000000. Compared with the responses of Alasino and the validated models, there exist reductions of 41% and 22% respectively. Such differences can be attributed to the employment of low value of and the shortened SRT. However, the cost for pumping energy increases from a base level of €149300 to €927000.

**Figure 6.7** Investment costs of three models

The variation in each sector of investment cost between three models is insignificant. The cost for tank construction in the optimal model design increases by 5% from €1744000 to €1820000. A decrease in the demand for dissolved oxygen leads to a slight reduction in the cost for aeration system, which is estimated as €122000. The cost for influent pumping station remains constantly at €269000. In addition, there is a slight increase in the cost for sludge recycle due to the increased recycle flow rate in the optimal design. In short, the cost for tank construction in three cases is the largest slice of the total investment cost and this value depends very much on two variables, the volume of reactor () and the inlet flow rate ().

Using the particle swarm algorithm the model yields a total plant cost (net present value) of €4270000, which is a third less than the values of the other two models. Saving €1400000 in the operating cost mainly arises from two sectors, the aeration energy and the sludge disposal. It is also found that a small value of SRT is more suitable for the activated sludge process due to the employment of fast growing biomass species. Moreover, nitrate produced in this system is more sensitive to the value of SRT. An increase in SRT will result in a decreased nitrate production. By placing an anoxic reactor at the front of the model configuration can improve the efficiency on carbon and nitrogen removal.

**6.3 Industrial WWTP Design and Synthesis under Steady State Conditions**

Since we validated the optimization methodology using a historic model, it has been found that the heuristic optimization methods in the form of particle swarm can yield more efficient solutions for design problems in wastewater treatment.

In this section, we focus on the use of particle swarm algorithm toaddress the simultaneous optimization of the process structure and operating conditions of wastewater treatment plants subject to a set of influent data including a year of inlet data at daily interval (dynamic state) and averaged inputs (steady state) given by an industrial wastewater treatment plant in China. We consider a three-unit model but allow the optimizer to determine the feed distribution and recycle rate. This is similar to the problem considered in chapter 4 but now with the detailed biochemical models in each of the process units. A steady state model with the default design parameters given in Table 6.9 is initially developed and simulated. The averaged influent flow rate and compositions (which are classified in an order of , , , , , , , , , , ,) are summarized in Table 6.8.

**Table 6.8** Averaged influent flow rate and compositions

|  |  |  |
| --- | --- | --- |
| Component | Concentration | Unit |
|  | 28.75 | g COD m-3 |
|  | 65.42 | g COD m-3 |
|  | 48.16 | g COD m-3 |
|  | 190.50 | g COD m-3 |
|  | 26.6 | g COD m-3 |
|  | 0 | g COD m-3 |
|  | 0 | g COD m-3 |
|  | 520 | g SS m-3 |
|  | 0 | g O2 m-3 |
|  | 0 | g N m-3 |
|  | 0 | g N m-3 |
|  | 37.58 | g N m-3 |
|  | 47087 | m3 d-1 |

**Table 6.9** Default design parameters

|  |  |  |
| --- | --- | --- |
| Design parameter | Default value | Unit |
|  | 20000 | m3 |
|  | 20000 | m3 |
|  | 20000 | m3 |
|  | 150 | d-1 |
|  | 150 | d-1 |
|  | 150 | d-1 |
|  | 1 | Na |
|  | 1 | Na |
| SRT | 20 | d |

Modelling of steady state systems is quiet common in practice as it can provide a reasonable prediction of plant performance. Considering the influent data displayed in Table 6.8, it is found that the characteristics of COD are quite similar to those used in the previous section for validating the optimization methodology, apart from the composition of volatile suspended solids (), which is, here, given as 520 g *SS* m-3. The initial design of the steady state model is configured with three equal-sized reactors, each of which is assigned a value of as 150 d-1. This is to ensure the sufficient quantities of dissolved oxygen in each unit for the growth of aerobes. A high value of hydraulic retention time is also guaranteed as the upper bound of reactor size is set as 20000 m3. The total inlet flow rate is given as 47087 m3 d-1. , as the coefficient of total flow rate, is set as 1. A recycle stream is also allocated which conveys the mixed liquor suspended solids from the last unit to the first reactor with the same flow rate as the total inlet. SRT in this process is chosen as 20 days. Table 6.11 displays the steady state simulation results determined using the default design parameters.

**Table 6.11** Steady state simulation results based on the default design parameters

|  |  |  |
| --- | --- | --- |
| Effluent | Concentration | Unit |
|  | 28.75 | g COD m-3 |
|  | 0.02 | g COD m-3 |
|  | 8.95 | g O2 m-3 |
|  | 43.7 | g N m-3 |
|  | 1.25 | g N m-3 |
|  | 0.03 | g N m-3 |

The concentrations of and are significantly reduced from their initial levels of 65.42 g COD m-3 and 37.58 g N m-3 to 0.02 g COD m-3 and 0.03 g N m-3in the effluent. Such sharp decreases are attributed to the sufficient supply of oxygen and the employment of high hydraulic retention time. However, a defect is realized that there is no venue for denitrification. In addition, the level of in the effluent, another target to be minimized, is computed as 43.7 g N m-3 which is well above the discharge limit and leads to an extremely high operating cost. To reduce the value of to a tolerant low level while minimizing the total plant cost, we apply the optimization methodology to the steady state model and the optimal solutions are determined and summarized in Table 6.12.

**Table 6.12** Optimal model results

|  |  |  |  |
| --- | --- | --- | --- |
| Effluent | Concentration | Design parameter | Optimal value |
|  | 28.75 g COD m-3 |  | 19988 m-3 |
|  | 0.06 g COD m-3 |  | 19995 m-3 |
|  | 2.75 g O2 m-3 |  | 6030 m-3 |
|  | 8 g N m-3 |  | 0 |
|  | 28.67 g N m-3 |  | 31.4 d-1 |
|  | 1.5 g N m-3 |  | 117 d-1 |
|  | 0 |
|  | 2.89 |
| SRT | 5.3 d |

The optimal effluent compositions appear to be more reasonable, as the level of is sufficiently reduced and controlled at 8 g N m-3 which meets its constraint set in the algorithm. It also maintains a removal rate of 99.9% for and 96% for respectively. The optimal design of the steady state model is illustrated in Figure 6.8.

47087 m3 d-1

19988 m3

Anoxic

6030 m3

= 117 d-1

Aerobic

136081 m3 d-1

1666 m3 d-1

45421 m3 d-1

19995 m3

= 31.4 d-1

Aerobic

**Figure 6.8** Optimal design of the steady state model

The optimal flowsheet (Figure 6.8) contains a series of three reactors, an anoxic reactor followed by two aerobic reactors. The volumes of the first two reactors approximately reaching their upper bounds are determined as 19988 m3 and 19995 m3 respectively. This implies that the biomass requires a longer hydraulic retention time to degrade the heavy loads of COD and nitrogen matter. The allocation of an anoxic reactor at the front of the process flowsheet allows the conduction of denitrification in order to maintain the oxidized nitrogen material leaving the effluent at a tolerant low level. The degradation of biodegradable COD and nitrogen material is expected to be achieved in the last two reactors in spite that there is a low value of employed in the second reactor. SRT, another tuned parameter, is associated with the sludge production. It is computed as 5.3 days, which is treated as a reasonable value to be used in the activated sludge process. The optimal value of parameter is determined as zero so that the feed is directly conveyed to the second reactor. Figure 6.9 below shows the comparison of total plant cost between the default design and the optimal design.

**Figure 6.9** Net present values of the model with default design parameters and the model with optimal solutions

There is a significant decrease in the net present value of the optimal model. It entirely saves €6350000 compared with that of the model with default design criteria. The cost for tank construction in the optimal design, accounting for the second largest proportion (32%) of the net present value, is determined as €2980000. It is €50000 less than that of the default design. A relatively shortened SRT employed in the optimal flowsheet results in a cut of €5670000 in sludge disposal. However, it still accounts for the largest expenditure sector compared to other units and its new estimated value is determined as €3410000. In addition, the sharp decrease in the cost for aeration energy demand is mainly attributed to the employment of low values of and its corresponding value is calculated as €439000. The expenditure on pumping energy in the optimal design increases due to the tripled recycle flow rate. It accounts for 18% of the total plant cost. The variations in the rest sectors between two models are not that evident. For example, the optimal cost for aeration device is computed as €178000 (2% of NPV), influent pumping station as €463000 (5% of NPV) and sludge recycle as €69719 (1% of NPV) respectively.

**6.3.1 Testing the Steady State Optimal Design Subject to Dynamic Inputs**

Steady state model optimization is usually treated as the end point of synthesis for most applications since the optimal design of steady state model can perform well when dealing with moderate influent data (i.e. constant feed). However, the fact is that plants in practice deal with varying inputs and many of those frequently failed in operation when treating wastewater under severe weather conditions. An additional check of the compatibility of the just-determined optimal design subject to the time-varying inputs provided by the plant is, thus, carried out. We compare the value of each NPV component when the optimal design of model subject to: 1. the averaged inputs and 2. the dynamic inputs. The corresponding results are displayed in Figure 6.11.

**Figure 6.11** NPV of two cases

The total NPV in case 2 is calculated as €26687000, which is about three times bigger than that in case 1**.** This huge difference (€17437000) is mainly attributed to a significant rise in the cost for sludge disposal in case 2 and this heavy burden on the operating costs is due to the accumulation of the concentrated particulates in reactors as well as the inappropriate SRT chosen that causes unstable sludge discharged from the system. Apart from this, both cases behave quiet similar as the costs for the rest units/processes are very close to each other.

The conclusion is that the use of design of steady state model to practical purposes is very limited as it yields a number of uncertainties in effluent quality when dealing with dynamic inputs with shock loads under severe weather conditions. Therefore, the development of a dynamic wastewater treatment model capable of treating a variety of input conditions as well as achieving a cost-effective design is very attractive. In the next part, we devote ourselves to the optimal design of wastewater treatment plants subject to time-varying inputs.

**Part : Optimal Design of WWTPs Subject to Time-Varying Inputs**

In part we demonstrated the optimal design of the steady state wastewater treatment plants based on the use of heuristic optimization in the form of the particle swarm algorithm. Here we consider the model optimization when subject to time-varying inputs. Our intention is to develop a cost effective process configuration that is capable of dealing with the large variations in influent.

**6.4 Variability of WWTP Loading**

Wastewater treatment plants are inherently dynamic because of the large variations in influent wastewater flow rate and compositions. To some extent, these variations are predictable, but not possible to control. Usually, hourly, daily or weekly variations are very likely to be observed when carrying out the analysis of water quality on plants. An example (Figure 6.12) below shows a 9-month period of daily influent COD compositions feeding to a wastewater treatment plant in China.

**Figure 6.12** A 9-month period of daily influent COD compositions to a wastewater treatment plant in China

As can be seen from Figure 6.12, the daily influent COD compositions to the plant vary significantly, especially the fluctuations appearing during the first 118 days with a number of local peaks (such as the peak 1 on day 49; the peak 2 on day 89; the peak 3 on day 113 and the peak 4 on day 118) which are well-above the averaged level. The fact is that wastewater treatment plants with fixed design dimensions are found to be very problematic in dealing with the incoming wastewater with such large fluctuations. A sudden increased flow rate leads to a dramatic decrease in the hydraulic retention time. This will narrow down the time for bacterial metabolism and result in an effluent with higher concentrations of pollutants. If high levels of such effluent are released unchecked into local watercourses, it can be a disaster for local communities.

As only 9 months of influent data (flow rate and wastewater compositions) was provided from the plant, we decided to supplement another 3 months data in order to make a year cycle for a complete data analysis in our dynamic model. This was done by repeating the last and the first one and half month of the existing data. Figure 6.13 displays a year cycle of daily influent COD compositions. Figure 6.14 shows the daily variations in the influent. The daily influent flow rate to the plant is illustrated in Figure 6.15

**Figure 6.13** A year cycle of daily influent COD compositions

In the absence of a comprehensive suite of analytical instruments operated in the plant, the analysis of the influent wastewater compositions is restricted to the measurement of the concentration of total COD. The concentrations of COD components shown in Figure 6.13 are calculated according to a fraction distribution (18.4% for , 13.4% , 53% , 7.4% and 7.8% ), which was used in the COST benchmark simulation for the analysis of steady-state treatment models.

Considering the daily variation of COD in Figure 6.13, it is evident that there is a sharp decrease in the concentration of total COD from 240 g COD m-3 on day 1 to 130 g COD m-3 on day 28, and then it reverses back to a peak value of 1142g COD m-3 on day 118 with a steep increase. A continuous drop lasting for 210 days afterward occurs and the lowest value of COD is detected as 130 g COD m-3 on day 1 and 338 respectively. After that, the trend rises again and stops at a value of 730 g COD m-3 on day 363. It could be assumed that the sharp increase in March to the level in mid of May presents the most challenge part for plant operations.

**Figure 6.14** Daily influent

There is a little difference in the trend of compared to that of total COD. In the first 100 days, the level ofkeeps moving up and down from a regional peak of 60.4 to a low of 26.6 g N m-3. A global peak for is found as 91.2 g N m-3 on day 179, and it then drops to a low at 13 g N m-3. After that, the values of are kept within an upper bound of 67.5 g N m-3 and a lower bound of 13 g N m-3.

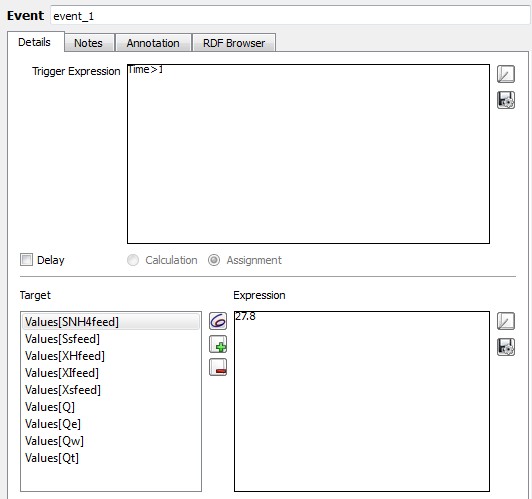
**Figure 6.15** Daily influent flow rate

The daily inlet wastewater flow rate displayed in Figure 6.15 is relatively stable, varying in a narrow range from 40000 m3 d-1 to 50000 m3 d-1 for most of the year, apart from a few extreme cases that scatter at different time spots as local/global minima on the graph. These points are separately marked as: = 33336 m3 d-1 on day 26, = 36667 m3 d-1 on day 126, = 33347 m3 d-1 on day 181, = 21401 m3 d-1 on day 261, and = 33336 m3 d-1 on day 338. Investigating model responses at these points against those at the moderate flow rates is of great interest.

**6.4.1 Modelling of Time-Varying Inputs (Flow Rate and Compositions)**

The ‘Events’ module in Copasi, which is used for simulating discrete parameter changes during the simulation, was used to model these time dependent inputs for the dynamic model. It consists of two key parts, namely: a *trigger*, which causes the event and at least one *assignment*, which allows a modification of the input data to the model (Copasi, 2010).

Each daily influent data set (including compositions and flow rate) is treated as a single event so that 365 events are formed. The order of each event is represented by the time inequality in the trigger expression (for example: time > 1 means the first event and time > 2 for the second event and so on). An event is only fired in the model simulation when its trigger expression changes from false to true. In addition, the feed to the model is explicitly defined in the assignment target box with their corresponding values displayed in the expression box. All assignments associated with a single event are executed as one unit. The ‘Events’ module in Copasi is displayed in Figure 6.16.

****

**Figure 6.16** ‘Events’ module in Copasi

**6.5 Modelling of Dynamic Systems Based on the Default Design Criteria**

To make an unbiased comparison with the steady state model, the same default design parameters given in Table 6.9 are used in this dynamic model. The process flowsheet also consists of three aerobic reactors in series and a sedimentation tank. The feed stream is distributed among the first two reactors and a recycle stream between the first reactor and the settler is linked.

Using the time course simulation based on the ordinary differential equation solver, the dynamic model defined as the differential equations in Copasi are solved. It achieves significant reductions in both COD and as shown in Figure 6.17 & Figure 6.18 respectively. Such great reductions are mainly attributed to the allocation of three aerobic reactors with large oxygen transfer coefficients. In addition, a high level of dissolved oxygen (Figure 6.19) in the effluent is found as 9 g O2 m-3. This is due to the applying of the high values of to all three reactors. However, due to the lack of anoxic unit employed in this process configuration, the model yields a large quantity of oxidized nitrogen compounds in the form of nitrate in the effluent, which is harmful to the ecosystem and the aquatic life.

**Figure 6.17** Simulation result -

**Figure 6.18** Simulation result -

**Figure 6.19** Simulation result -

**6.6 Dynamic Model Optimization**

Applying either deterministic or heuristic optimization algorithms to dynamic models to work out appropriate optimal design solutions is time-consuming. Furthermore, the more events to analyze, the longer the dynamic simulation takes since the integrator must take smaller steps in time due to the finer time resolution. This therefore serves to increase running times, although it does not directly increase the complexity of the optimization problems by increasing the number of decision variables.

Implementing the particle swarm on the dynamic model, the optimal solutions are summarized in Table 6.13 and the optimal flowsheet is displayed in Figure 6.21. The solutions are non-rigorously described as ‘optimal’ in the sense of the best found although better solutions could exist.

**Table 6.13** Optimal solutions of the dynamic model

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Parameter | Optimal value | Starting value | Lower bound | Upper bound |
| (m3) | 270 | 20000 | 0 | 20000 |
| (m3) | 18056 | 20000 | 0 | 20000 |
| (m3) | 19999 | 20000 | 0 | 20000 |
| (d-1) | 119 | 150 | 0 | 150 |
| (d-1) | 84 | 150 | 0 | 150 |
| (d-1) | 0 | 150 | 0 | 150 |
|  | 0.65 | 1 | 0 | 1 |
|  | 2.85 | 20 | 0 | 20 |
| SRT (d) | 1.86 | 30 | 0 | 30 |

18056 m3

= 84 d-1

19999 m3

Anoxic

, =2.85

270 m3

=119 d-1

**Figure 6.21** Optimal design of the dynamic model subject to 365 events

The feed in this flowsheet has been distributed among the first two reactors with an optimal value of as 0.65. There is no significant change on selection of the equipment type in this configuration, but the allocation of reactors is in an order of an aerobic reactor followed by another aerobic and then by an anoxic reactor. The values of in the first two reactors are determined as 119 d-1 and 84 d-1 respectively. In addition, there is a sharp decrease in the optimal SRT which comes out as 1.86 d and the recycle coefficient is determined as 2.85. It believes that such a low value of SRT used in this optimal design is adequate for the biomass to carry out the essential metabolic reactions while providing a stable effluent quality. This also ensures a lower operating cost for the sludge disposal. The corresponding model responses in terms of effluent COD and are displayed in Figure 6.22 and 6.23 respectively. Figure 6.24 shows the net present value of the optimal dynamic model.

**Figure 6.22** Dynamic simulation result -

In terms of removal, this dynamic model with the optimal design performs very well despite the fact that there is a sharp peak at the beginning of simulation. This abnormal phenomenon is due to the great difference between the starting point value and the input of the first event thus misleading the deterministic algorithm to find a few significantly fluctuated solutions during the simulation. These results are thus not taken into consideration in the effluent quality analysis. The concentration of the readily biodegradable COD in the following events is maintained at an average level of 0.2 g COD m-3, with a peak value of 20 g COD m-3 at the 118th day and a lowest point of 0.05 g COD m-3 at the 28th day.

**Figure 6.23** Dynamic simulation result -

The same problem of a sudden increase and then a decrease also appears to the nitrogen degradation. As a common technical problem, it can be ignored in the following data analysis. A high removal rate is achieved in this case and its average value is determined as 1.3 g N m-3, which is significantly lower than its threshold value which is 4 g N m-3 (Table 2.6). Apart from a few peaks (such as = 24.4 g N m-3, =14.7 g N m-3 and =25.6 g N m-3) detected during a period from day 109 to day 183, the in most time of the year maintains at a level around 0.4 g N m-3, which is even lower than the initial constraint attached on the optimization problem.

**6.6.1 The Challenge of Minimizing Accumulated Costs in Copasi**

There is a challenge encountered when optimizing the dynamic model which consists of 365 events. The optimizer used in Copasi under time-course subtask is merely applicable to the value of the variables at the final time of the simulation, whereas we want to minimize the total accumulated costs over the whole year. The use of the total plant cost expression (Equation 6.9) of the steady state model is thus inadequate for the dynamic model. We, therefore, use a dummy reaction to formulate a cumulative function (Equation 6.11) as the objective function which accumulates the daily plant costs is based on the output variables pertaining at each event. The optimizer solves the objective function containing the sum of the fixed investment costs and the summed operating costs to find the best trade-off between them. The best solution for the minimum total plant cost is thus determined and is displayed in Figure 6.24. Table 6.14 below summarizes the net present value expressions used in the steady state and the dynamic models.

**Table 6.14** Objective functions for the steady state and the dynamic models

|  |  |
| --- | --- |
| Model optimization | Objective function |
| Steady state model |  |
| Dynamic model |  |

There are two implicit assumptions in the formulation of the dynamic cost objective function.

First, since we only have a daily time varying data for a 12 month period, we are assuming that the same annual pattern is repeated over the lifetime of the plant. This is clearly very unlikely, but it is reasonably assumed that the daily data used is indicative of the degree of variability over an average year.

Secondly, since we are using a dynamic simulation which reports model variables at an arbitrarily fine time granularity (e.g. in principle, down to the nearest second), we are assuming that the value of each model variable at the end of each day is close to its value over the whole of the preceding 24 hours. This is a reasonable assumption since the perturbations we are making to the system are daily and intrinsic model dynamics are quite slow (i.e. days or weeks). The model outputs do not, therefore, change very much over the course of 24 hours and the value of each state variable at the end of each day can be accurately assumed to be the value that pertains over the whole day.

Cumulative NPV = €8640000

**Figure 6.24** Net present values of the optimal design of the dynamic model

As expected, there is a monotonic rise in the cumulative net present value from zero at the starting point of the simulation to a sum of €8640000 at the last event. This value is treated as the minimum total plant cost of the dynamic model, which is further used for a comparison with the optimal NPV determined in the steady state model in the following section.

**6.7 Optimal Design Comparison between the Steady and Dynamic State Models**

To ensure an unbiased comparison, we initially simulated a steady state model and a dynamic model based on the same default design criteria respectively. Implementing the particle swarm algorithm on both models we achieved different sets of optimal solutions. A diagrammatic comparison of NPV between two models is displayed in Figure 6.25.

Compared to the optimal design of the steady state model, the dynamic one yields €614000 less in terms of net present value. This is equivalent to a cost saving of 5% and such a difference is mainly attributed to the following factors including: the savings on the tank construction (€57000), the aeration system (€27000), the pumping energy (€23480) and the sludge disposal (€170000). However, due to the specific requirement to maintain a high removal rate for COD and nitrogen, the cost for aeration energy used increases by €160000 in the dynamic model as compared to the steady state model. The differences between other units among two models, such as the sludge recycle and the pumping station, are too small to consider.

**Figure 6.25** Net present values of two models

Figure 6.26 displays the distribution of the net present value of the optimal dynamic model. It can be seen that the sludge disposal operating cost, the tank construction investment cost and the pumping energy operating cost are the three main contributors to the overall project cost (net present value).

**Figure 6.26** Cost distributions

**6.8 Computational Aspects**

As a final remark the computational effort is considered. This is one of the major aspects to evaluate the performance of optimization algorithms/models. The optimization models (both the steady state model and the dynamic model) in this chapter are implemented in Copasi and solved using the particle swarm with 100 iterations and a swarm size of 50. According to the computational statistics shown in Table 6.15, the total CPU time needed to solve the dynamic optimization model is approximately 40.64 hours on an Intel Core i-3 of 2.4GHz with 4 GB of RAM. However, solving the steady state one only takes one hour. Such a significant difference in CPU time between two models is mainly attributed to the number of events involved in the optimization problem. The steady state model includes only one event and the determined optimal parameters merely deal with the compositions in that event. However, the algorithm in the dynamic model takes more time searching for optimal parameters for 365 events and result in a set of parameters that is capable of dealing with the time-varying inputs over the course of a year.

For practical use the modification of the optimization algorithm will have to be required in order to reduce the computational time. To this end, two tasks can be considered and explored in the future: reduction of plant model dimension and reduction of optimization parameters.

**Table 6.15** Required CPU time to optimize the steady state model subject to averaged input (1 event) and the dynamic model subject to time-varying inputs (365 events)

|  |  |
| --- | --- |
| Model type | CUP time (h) |
| Steady state model | 1 |
| Dynamic state model | 40.64 |

**6.9 Summary**

In this chapter, we have developed a mathematical framework for optimal design of wastewater treatment plants that simultaneously takes into account the dynamic variations in both flow rate and compositions. A subsequent comparison of the plant performance with respect to the steady state design is carried out. The key findings are summarized as follows:

* The initial rebuilding of Alasino’s model demonstrates a good validation of our design methodology (e.g. our model yields removal rates of 99.4% and 99.9% for and Alasino’s model achieves 98.4% and 99.9%). However, a perfect match between each component of solids can not be determined as our method is assumed to have a perfect separation in the simulation flowsheet, whereas Alasino, who uses a model of the secondary clarifier, does not.
* With given a year of influent data at daily interval sampled in an industrial wastewater treatment plant in China, a treatment plant with nominal design parameters is designed, simulated and optimized under both steady state and dynamic state conditions. We further compare the performance of both scenarios and demonstrate that the optimal design of the steady state model when taking the daily varying inputs into considerationis sub-optimal as compared to our novel design method (the dynamic one) that explicitly takes into account the varying inputs. In addition, according to the results shown in Table 6.16, a high level of total nitrogen is yielded in the effluent using the steady state model as 10.2 g N m-3,which is well above both the threshold value (4 g N m-3) and the value determined in the dynamic model (1.3 g N m-3). Furthermore, the total plant cost using the steady state design is extremely large and is three times greater than that by the dynamic one. Such a significant difference is mainly attributed to a sharp increase in the cost of the sludge disposal when dealing with high loaded suspended solids. Given that it is more confident to reveal the superiority of our design method in dealing with fluctuated inputs while minimizing total plant costs.

**Table 6.16** Performance of the steady state and dynamic state models when subject to the time-varying inputs

|  |  |  |
| --- | --- | --- |
| Effluent | The performance of the optimal steady-state model subject to the dynamic inputs | The performance of the optimal dynamic-state model |
|  | 0.3 g COD m-3 | 0.2 g COD m-3 |
|  | 10.2 g N m-3 | 1.3 g N m-3 |
|  | 8 g N m-3 | 22 g N m-3 |
| Cost |  | |
| Operating cost (over a plant life span of 20 years) (€) | 23000000 | 5540000 |
| Investment cost (€) | 3690000 | 3100000 |
| Total net present value (€) | 26690000 | 8640000 |

1. **Conclusions and Future Works**

In this thesis, we have demonstrated an optimization methodology that addresses the simultaneous optimization of process design and operating conditions of large-scale wastewater treatment plants for organic carbon and nitrogen removal. Due to the dynamic characteristics of industrial plants, this attempt, for the first time, takes dynamic variations in both feed compositions and flow rate into consideration as a part of model optimization rather than most cases relying on averaged inputs.

The contributions of this work can be concluded in three parts, namely: modelling, optimization and application.

* **Modelling**: We have developed a process model coded in system biology markup language (SBML) that can be shared between freely available tools such as CellDesigner, Sentero, Copasi. This model utilizes a methodology for process synthesis and enables consideration of dynamic inputs. It allows other users to investigate our model and allows us to apply the suite of powerful analysis and optimization algorithms provided by these tools.
* **Optimization:** We have presented a comprehensive comparison of a range of optimization algorithms to assess their efficiencies in solving the nonlinear process synthesis of the minimum wastewater treatment model. In terms of the accuracy of optimal solutions and the expense of computation, the particle swarm algorithm, has been selected as the most effective means. We have also validated our optimization methodology with respect to the historic model design configuration determined by Alasino using MINLP. This validation involves the comparisons of effluent quality and net present value between two models. Our approach yielded an even lower net present value for the plant.
* **Application:** We have applied the methodology to an industrial scale wastewater treatment plant and carried out a comparison between the novel dynamic design approach and the averaged steady state approach. The results show that the optimal design of the steady state model when taking the daily varying inputs into consideration is proved to be sub-optimal as compared to the dynamic design. Its estimated total plant cost is much greater than that of the dynamic model. We have also investigated the optimal performance of the same industrial plant by adding a physical retrofit to the existing configuration using a specialized commercial software tool. The allocation of two anaerobic digesters leads to 8000kWh power recovery in the plant everyday due to the generated methane and a 2/3 of total energy is saved.

**Future Works**

Regarding the results that have been presented, it is of necessity to state some limitations of our approach and the extensions that need to be considered in the future. More detailed information is summarized as follows:

* Development of better settler models: Having assumed a perfect separation in our modelling approach all generated suspended solids were expected to be recycled back to the reactor or disposed as waste sludge. We thus achieved a high quality effluent that only contains soluble components. However, this finding is not truly reflected in reality as there should be a small fraction of particulate together with soluble components leaving in the effluent. Adding an appropriate sized settler model to our approach is of necessity as it can provide an accurate prediction of sludge separation. A one-dimensional layer model is thus considered. This model is a two-step procedure that simultaneously deals with the clarification of mixed liquor suspended solids and the thickening of sludge in the settler. Therefore, particulate and soluble component balance equations are defined separately. In addition, due to the non-smooth nature of functions defined in settler models, there may or may not be some numerical problems (e.g. discontinuities) when applying derivative-based optimization methods to settler models.
* Development of aerobic digestion models using general-purpose software tools: in chapter 5 we demonstrated the ability of energy recovery of anaerobic digestion model. However, this was done using a commercial software tools (BioWin), which has many technical limitations. For example, BioWin strictly prohibits modellers from modifying some essential parameters/variables of selected process models. It is, therefore, difficult to get insight into the interaction between reactants and products and the investigation of the effect of parameters on model performance is not feasible. It is of necessity to develop anaerobic digestion models using self-coded software tools so that the models can be manipulated to maximize the production of methane in order to improve plant performance.
* Expanding the scope of modelling target (e.g. taking phosphorous removal into consideration): phosphorous and nitrogen are the major nutrients to be removed from treated wastewater. Adding the mechanism of phosphorous removal to our existing model would perfect its performance to the realistic target features. However, the difficulty would be the integration of the kinetics of phosphorous removal to our model because of the consideration of more state variables (including microbiological species and phosphorous compositions) and reactions. This would complicate simulation and optimization.
* Making our model more comprehensible and ease to use: the continuous improvements in wastewater treatment models, to some extent, enhance the accuracy in performance prediction. This, however, complicates the model structures due to the consideration of additional variables. To make our model more comprehensible and easy to use, we have to focus on the development of an alternative way of eliminating some parameters that have minor effects on model outcomes. The integration of ASM with TUDP models can significantly reduce the number of irrelevant parameters involved, while maintaining the mechanistic structure. This integrated model can also provide a deep insight into the mechanisms of phosphorous removal and denitrification.

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1. **Appendix**

**9.1 Typical Values of Kinetic Parameters for ASM3**

**Table 9.1:** typical values of kinetic parameters for ASM3

|  |  |  |  |
| --- | --- | --- | --- |
| Symbol | Characterization | Temperature  20oC | Unit |
|  | Hydrolysis rate constant | 3 | g (g )-1d-1 |
|  | Hydrolysis saturation constant | 1 | g (g )-1 |
| *Heterotrophic organism , aerobic and denitrifying activity* | | | |
|  | Storage rate constant | 5 | g (g )-1d-1 |
|  | Anoxic reduction factor | 0.6 | - |
|  | Saturation constant for | 0.2 | g O2 m-3 |
|  | Saturation constant for | 0.5 | g m-3 |
|  | Saturation constant for | 2 | g m-3 |
|  | Saturation constant for | 1 | g (g )-1 |
|  | Heterotrophic max growth rate of | 2 | d-1 |
|  | Saturation constant for ammonium, | 0.01 | g N m‑3 |
|  | Saturation constant for alkalinity for | 0.1 | Mole m-3 |
|  | Aerobic endogenous respiration rate of | 0.2 | d-1 |
|  | Anoxic respiration rate of | 0.1 | d-1 |
|  | Aerobic respiration rate for | 0.2 | d-1 |
|  | Anoxic respiration rate for | 0.1 | d-1 |
| Autotrophic organisms , nitrifying activity | | | |
|  | Autorophic max growth rate of | 1 | d-1 |
|  | Ammonium substrate saturation for | 1 | g N m-3 |
|  | Oxygen saturation for nitrifiers | 0.5 | g O2 m-3 |
|  | Bicarbonate saturation for nitrifiers | 0.5 | mole m-3 |
|  | Aerobic endogenous respiration rate of | 0.15 | d-1 |
|  | Anoxic endogenous respiration rate of | 0.05 | d-1 |