DOKUZ EYLÜL UNIVERSITY
GRADUATE SCHOOL OF NATURAL AND APPLIED SCIENCES

MATHEMATICAL MODEL APPLICATIONS OF ACTIVATED SLUDGE

by
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February, 2006
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MATHEMATICAL MODEL APPLICATIONS OF ACTIVATED SLUDGE

A Thesis Submitted to the
Graduate School of Natural and Applied Sciences of Dokuz Eylül University
In Partial Fulfillment of the Requirements for the Degree of Master of Science
in Environmental Engineering, Environmental Technology Program

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M.Sc. THESIS EXAMINATION RESULT FORM

We have read the thesis entitled **"MATHEMATICAL MODEL APPLICATIONS OF ACTIVATED SLUDGE"** completed by **Mehmet Bedrettin KÖSE** under supervision of **Prof. Dr. Davut ÖZDAĞLAR** and we certify that in our opinion it is fully adequate, in scope and in quality, as a thesis for the degree of Master of Science.

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ACKNOWLEDGEMENTS

I would like to express my sincere gratitude to my supervisor, Prof.Dr. Davut ÖZDAĞLAR for his valuable advices and guidance, Prof.Dr. İbrahim ALYANAK who shared his time and knowledge with me, M.Sc Env. Eng. Elif Ceyda TORCU who first gave me the idea on the concept of this study.

I am also grateful to my mother for her understanding and endless support throughout this study.

M. Bedrettin KÖSE

MATHEMATICAL MODEL APPLICATIONS OF ACTIVATED SLUDGE

ABSTRACT

Application of mathematical models in design and operation of biological nutrient removal systems is becoming more important with the legislations getting stricter. Recent developments in computer technology enabled development of computer programs that are able to solve complex models required to describe the processes taking place in activated sludge plants. In this study, several methods for determining COD and nitrogen fractions and kinetic and stoichiometric parameters for domestic wastewaters are evaluated, and wastewater is fractionated using actual plant measurements and results of previous studies in literature. In addition, IWAQ Activated Sludge Model Number 1 (ASM1) is applied to İzmir Güneybatı Wastewater Treatment Plant using Single-sludge Simulation Program (SSSP) as the simulation environment. Default kinetic and stoichiometric parameters offered by IWAQ Task Group are used in simulations. Simulation studies are performed with different COD concentrations to determine plant's organic capacity. As a result of study, it is shown that the fate of carbonaceous and nitrogenous components of wastewater and MLSS concentration in aeration tanks can be successfully simulated and plant's response to various conditions can be estimated using ASM1.

Keywords: Modeling, ASM1, COD fractionation, SSSP, simulation

AKTİF ÇAMURDA MATEMATİKSEL MODEL UYGULAMALARI

ÖZ

Giderek sıkılaşan yasal düzenlemelerle birlikte biyolojik nutrient giderimi sistemlerinin tasarımı ve işletiminde matematiksel model uygulamaları önem kazanmaya başlamıştır. Bilgisayar teknolojisindeki gelişmeler aktif çamur tesislerinde devam eden süreçlerin açıklanabilmesi için gerekli olan kompleks modelleri çözebilen bilgisayar programlarının geliştirilebilmesini sağlamıştır. Bu çalışmada, evsel atıksularda KOI ve azot fraksiyonları ile kinetik ve stokiyometrik parametrelerin belirlenmesinde kullanılan metodlar değerlendirilmiş, atıksu gerçek tesis verileri ve literatürde bulunan çalışma sonuçları kullanılarak fraksiyonlarına ayrılmıştır. Ayrıca, "IWAQ Activated Sludge Model Number 1 (ASM1)" modeli, "Single-sludge Simulation Program (SSSP)" programı kullanılarak İzmir Güneybatı Atıksu Arıtma Tesisi'ne uygulanmıştır. Simülasyonlarda, modeli geliştiren IWAQ Çalışma Grubu tarafından önerilen kinetik ve stokiyometrik parametreler kullanılmıştır. Tesisin organik kapasitesinin belirlenmesi amacıyla farklı KOI konsantrasyonlarıyla simülasyon çalışmaları yapılmıştır. Çalışma sonucunda, gerek karbonlu ve azotlu maddelerin gideriminin, gerekse havalandırma havuzlarındaki MLSS konsantrasyonunun ASM1 kullanılarak modellenebildiği ve tesisin organik kapasitesinin tahmin edilebildiği belirlenmiştir.

Anahtar sözcükler: Modelleme, ASM1, KOI fraksiyonları, SSSP, simülasyon

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CHAPTER ONE
INTRODUCTION

One of the most widespread biological wastewater treatment techniques is the activated sludge process. In this process, a bacterial biomass suspension is responsible for the removal of pollutants. Depending on the design and the specific application, an activated sludge wastewater treatment plant can achieve biological nitrogen removal and biological phosphorus removal, besides removal of organic carbon substances.

As the environmental legislations imposing stricter effluent standards, more complicated methods for design, operation and control of wastewater treatment plants are needed. As a result, mathematical models have been developed and widely used to assist design and operation of wastewater plants. Advances in computer science have also enabled complicated mathematical models developed for the design of such complex systems. Computer simulations have been shown to mimic the behavior and predict the performance of full-scale plants with reasonable accuracy. With computer simulations, it is now possible to test alternative operational strategies for full-scale plants without going through laboratory studies on pilot plants. Moreover, computer simulations have also been widely used in optimization studies that lead to cost-effective operational strategies, for trouble-shooting and upgrading of existing biological treatment plants (Tchobanoglous & Burton, 2003; Xu & Hultman, 1996).

The increased knowledge about the mechanisms of different biological processes taking place in an activated sludge plant was translated into dynamic models that were developed to describe the degradation processes in the activated sludge plant. This study focuses on the Activated Sludge Model No. 1 (ASM1) (Henze *et al.*, 1987), which through the years has been the state-of-the-art model for activated sludge plants with biological nitrogen removal.

Calibration of ASM1 is a must step as it is for all mathematical models. Behavior of an activated sludge plant depends upon a large number of kinetic and stoichiometric parameters. In addition to kinetic and stoichiometric parameters, there are a number of parameters that specify influent characteristics of wastewater.

Fortunately most of these parameters are not very sensitive and do not change appreciably for systems treating different municipal wastewaters (Henze et al., 1987; Kappeler & Gujer, 1992; Xu & Hultman, 1996; Sin, 2000). Default values for majority of these parameters are derived from earlier studies. Influent wastewater fractions also change significantly from wastewater to wastewater and it is often necessary to characterize wastewater on a case basis.

General aim of this study is to determine wastewater fractionation in İzmir Güneybatı Wastewater Treatment Plant and to calibrate, test and apply ASM1 model for the plant.

CHAPTER TWO
THEROTICAL BACKGROUND

Activated sludge process is a typical aerobic suspended growth system for biological wastewater treatment, and has been used extensively in its original form as well as in many modified forms (Tchobanoglous & Burton, 2003). Operationally, wastewater treatment with the activated sludge process is typically accomplished using a flow diagram similar to the one shown in Figure 2.1.

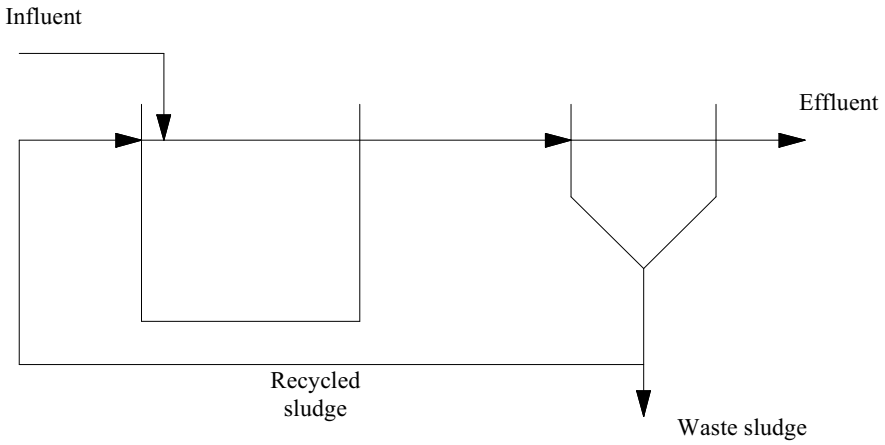

Figure 2.1 Schematic representation of activated sludge process (adapted from Tchobanoglous & Burton, 2003).

Organic waste is introduced into a reactor where an aerobic bacterial culture is maintained in suspension. The reactor contents are referred to as the "mixed liquor". In reactor, mixed liquor suspended solids (bacterial culture) decomposes and converts the biodegradable fractions of organic waste in generalized stoichiometric equation indicated below (Tchobanoglous & Burton, 2003).

$$COHNS + O_2 + \text{nutrients} \xrightarrow{\text{biomass}} CO_2 + NH_3 + C_5H_7NO_2 + \text{end products} \quad (2.1)$$

Stoichiometry indicated in equation (2.1) represents the general oxidation and synthesis of bacterial culture. Where COHNS refers to organic matter in wastewater and $C_5H_7NO_2$ represents cells produced in the reactor.

Generalized endogenous respiration reaction is written as follows:

$$C_5H_7NO_2 + O_2 \xrightarrow{\text{biomass}} 5CO_2 + 2H_2O + NH_3 + \text{energy} \qquad (2.2)$$

Although the endogenous respiration reaction results in relatively simple end products and energy, stable organic end products are also formed.

2.1 Biological Nitrification & Denitrification Processes:

Biological nitrification and denitrification are achieved by passing wastewater through simultaneous anoxic and aerobic steps. Biological denitrification is the process where nitrogen present in wastewater is considerably converted to nitrate. Unlike carbon oxidation, nitrification is an autotrophic process where energy required for biological growth is provided by oxidation of nitrogen compounds. The carbon source required for the synthesis of new cell is derived from inorganic carbon.

Main nitrogen form in domestic wastewater is ammonium nitrogen. The nitrification of ammonium nitrogen is a two-step process believed to involve two genera of microorganisms, nitrosomonas and nitrobacter. In the first step, ammonium is converted into nitrite and in the second step nitrite is converted to nitrate. (Tchobanoglous & Burton, 2003)

Denitrification is accomplished via denitrifying microorganisms that reduce inorganic nitrogen to the nitrogen gas under anoxic conditions. As denitrification is a heterotrophic process, organic carbon is used both as energy and carbon source for microbial growth. The ultimate goal in denitrification is to convert the nitrate nitrogen to any of the gaseous end-products and generally to nitrogen gas. (Tchobanoglous & Burton, 2003)

Denitrification process is highly susceptible to dissolved oxygen concentration in the reactor. If oxygen is present in the medium, anoxic respiration (denitrification)

terminates and the metabolic activity switches to aerobic respiration. To achieve an effective denitrification, oxygen concentration in the reactor should be maintained at near zero (Orhon & Artan, 1994).

2.2 Reactor Hydraulics

To simulate an activated sludge process, it is necessary to couple reactor hydraulics with reaction kinetics. Reactor hydraulics should be taken into consideration in order to simulate an activated sludge process.

Biological suspended growth reactors can be classified into two classes under consideration of operational modes: batch reactors and continuous reactors. Typically a batch reactor is operated on fill & draw basis. First the reactor is filled with all components of the processes and then the processes are allowed to react at constant volume. Any further mass input or output is prevented in this phase. After a specified time period long enough to achieve required process efficiency, reaction is stopped and reactor is decanted for the next cycle. On the contrary, continuous reactors receive influent and produce effluent continuously. (Orhon & Artan, 1994)

Batch reactors and common continuous reactor types used in suspended growth biological wastewater treatment processes are discussed under the next four subtitles.

2.2.1 Batch Reactors

As mentioned in previous paragraphs, there is no mass input and output to the batch reactor while the reaction continues. Therefore, the time-variant material balance is established as follows (Tchobanoglous & Burton, 2003):

Accumulation = Inflow – Outflow + Generation (2.3)

$$\frac{dC}{dt}V = QC_0 - QC + rV \quad (2.4)$$

where; C = concentration of the material in the reactor at time, t, M/L^3

C_0= initial concentration of the material in the reactor at time t= 0, M/L^3

V= reactor volume, L^3

Q= flowrate to the reactor, L^3/T

r= reaction rate of each process component in the reactor, M/L^3T

In a batch reactor, Q = 0, therefore, equation (2.4) can be reduced into a simpler form:

$$\frac{dC}{dt}V = rV \tag{2.5}$$

Reaction rate can be defined as $r = -kC^n$, where k is the reaction rate constant and n is the order of reaction. Then, the following integration is obtained by setting the limits $C = C_0$ for t = 0 and C = C for t = t:

$$\int_{C_0}^{C} -\frac{dC}{kC^n} = \int_0^t dt = t \tag{2.6}$$

When the reaction rate is under first order kinetics, the resulting expression becomes:

$$C = C_0 e^{-kt} \tag{2.7}$$

2.2.2 Completely Mixed Reactors

Once a particle enters in a completely mixed reactor, its concentration is assumed to be same throughout the reactor and in the effluent stream. If the reaction kinetics is first order, i.e. r = - kC, a time variant material balance equation for the reactive constituent C, in a completely mixed reactor can be established as follows, similar to equation (2.4) (Tchobanoglous & Burton, 2003):

$$\frac{dC}{dt}V = QC_0 - QC - kCV \tag{2.8}$$

The above equation can be simplified further by assuming steady-state conditions where accumulation of the reactive constituent does not occur. Under steady-state conditions, the derivative of the accumulation term becomes zero and equation (2.8) becomes:

$$0 = QC_0 - QC - kCV \tag{2.9}$$

Solving equation (2.9) for the reactive constituent, C, the following result that explains first order kinetics in a completely mixed reactor under steady-state conditions, is obtained:

$$C = \frac{C_0}{1 + k\left(\frac{V}{Q}\right)} \tag{2.10}$$

2.2.3 Plug Flow Reactors

In plug flow reactors, it is assumed that no mixing occurs in the axial direction and ideal mixing conditions are present in the radial direction. In other words, a differential volume, ΔV, represented by a length, Δx, along the reactor has the same mixing characteristics with the completely mixed reactors. This volume has no interaction with the next fraction and behaves like an individual completely mixed reactor.

For the differential volume element ΔV, the time-variant materials balance on reactive constituent is established as follows (Tchobanoglous & Burton, 2003):

$$\frac{\partial C}{\partial t}\Delta V = QC_x - QC_{x+\Delta x} + r\Delta V \tag{2.11}$$

Substituting the differential form of QC_x and $QC_{x+\Delta x}$ and $A\Delta x$ for ΔV yields the following expression:

$$\frac{\partial C}{\partial t} A\Delta x = -Q\frac{\Delta C}{\Delta x}\Delta x + rA\Delta x \tag{2.12}$$

Dividing both sides of equation (2.12) by A and Δx, following expression is obtained:

$$\frac{\partial C}{\partial t} = -\frac{Q\Delta C}{A\Delta x}\Delta x + r \tag{2.13}$$

Applying the steady-state conditions (i.e. $\partial C / \partial t = 0$) and taking the limit as Δx approaches zero, equation (2.13) becomes:

$$0 = -\frac{Q}{A}\frac{\partial C}{\partial x} + r \tag{2.14}$$

Integrating equation (2.14) after establishing the integration limits as $C = C_0$ for $x = 0$ and $C = C$ for $x = L$ and defining the rate of reaction as rkC^n, following expression is obtained (Tchobanoglous & Burton, 2003):

$$\int_{C_0}^{C} \frac{dC}{kC^n} = -\frac{A}{Q}\int_0^L dx = -\frac{A}{Q}L = -\frac{V}{Q} = \tau \tag{2.15}$$

where τ is the hydraulic retention time. This equation is the steady-state solution of the material balance for plug flow reactors without axial dispersion.

For n = 1, the solution of equation (2.15) will yield the similar result with the one obtained in batch reactor except for the concept for time:

$$C = C_0 e^{-k\tau} \tag{2.16}$$

2.2.4 Completely Mixed Reactors in Series

Completely mixed reactors in series are widely used reactors in wastewater treatment as they increase efficiency of some processes and have certain treatment advantages. Furthermore the output from a plug flow reactor with axial dispersion is often modeled using a number of completely mixed reactors in series. The hydraulic properties of completely mixed reactors in series also differentiate from their individual characteristics (Tchobanoglous & Burton, 2003).

Assuming a pulse input with a concentration of C_0 into a number of (i.e. n) equally sized completely mixed reactors in series with a total volume of V, the volume of each reactor will be V / n. Writing the material balance for the second reactor results:

$$\frac{V}{n}\frac{dC_2}{dt} = QC_1 - QC_2 \tag{2.17}$$

The effluent concentration from the first reactor is calculated using equation (2.7):

$$C_1 = C_0 e^{-n(Q/V)t} = C_0 e^{n\theta} \tag{2.18}$$

Substituting this equation into equation (2.17) and rearranging yields:

$$\frac{dC_2}{dt} + \frac{nQ}{V}C_2 = \frac{nQ}{V}C_0 e^{-n\theta} \tag{2.19}$$

At steady-state conditions, above equation is simplified as:

$$C_2 = C_0 n\theta e^{-n\theta} \tag{2.20}$$

The generalized equation for the effluent concentration of the i^{th} reactor in a series of n reactors is:

$$C_i = \frac{C_0}{(i-1)!}(n\theta)^{i-1}e^{-n\theta} \qquad (2.21)$$

2.3 Reaction Kinetics

On a modeling basis, reaction kinetics involves two basic processes; microbial growth and decay (Orhon & Artan, 1994). As process Stoichiometry interrelates substrate utilization with microbial growth, these two processes are studied together. Although microbial decay is defined as the decrement in biomass, in latter approaches it's understood that other effects of microbial decay such as degradation of biomass into substrate, must be taken into consideration (Henze *et. al.*, 1987). In Figure 2.1, combined effect of these two processes is shown in a closed system with no initial substrate limitation.

As seen on Figure 2.2, adaptation phase, followed by rapid growth phase is observed in a biological reactor under aerobic conditions. Third growth phase is the stationary phase which microorganisms reach the maximum growth rate. Finally, as a result of decreasing substrate concentration and inhibitory effect of accumulating metabolic products, growth rate of microorganisms decreases.

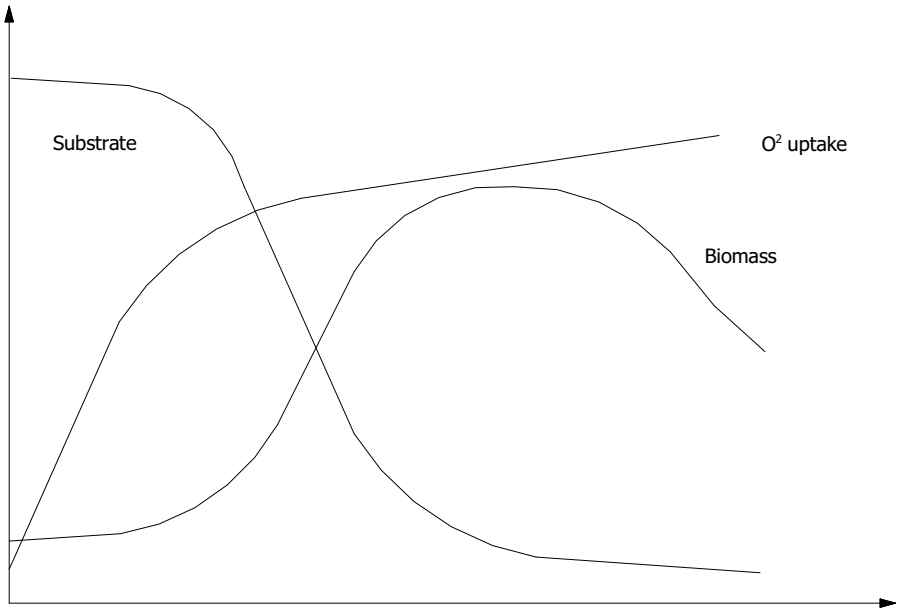

Figure 2.2 Biomass growth and decay, substrate removal and oxygen utilization under aerobic conditions. (Tchobanoglous & Burton, 2003)

Subsequently, a stationary phase where the endogenous metabolism is under equilibrium with synthesis of new cells. Reactions end with an endogenous phase where endogenous metabolism dominates because of substrate limitations (Orhon & Artan, 1994).

2.3.1 Microbial Growth

Microbial growth is usually defined with the following expression (Orhon & Artan, 1994):

$$\frac{dX}{dt} = \mu X \tag{2.22}$$

where; X= biomass concentration [M(biomass)/L^3]

μ= specific growth rate [T^{-1}]

Growth can also be defined in terms of substrate removal with a yield term:

$$\frac{dX}{dt} = -Y\frac{dS}{dt} \tag{2.23}$$

Hence, the relationship between substrate removal and microbial growth is:

$$\frac{dS}{dt} = -\frac{\mu}{Y}X \tag{2.24}$$

Specific substrate removal rate, q, is related to substrate removal in the following expression:

$$\frac{dS}{dt} = -qX \tag{2.25}$$

Thus, in terms of specific growth rate, q equals to:

$$q = \frac{\mu}{Y} \tag{2.26}$$

The relationship between maximum specific growth rate and growth-limiting substrate concentration is usually explained using the Monod equation, which named after Jacques Monod, who first demonstrated the fit of μ to S in accord with the rectangular hyperbola (Tchobanoglous & Burton, 2003; Orhon & Artan, 1994).

$$\mu = \hat{\mu}\frac{S}{K_S + S} \tag{2.27}$$

where; S= rate-limiting substrate concentration [M(substrate)/L^3]

μ= maximum specific growth rate [T^{-1}]

K_S= half-saturation constant [M(substrate)/L^3]

Substituting μ in equation (2.27) in equations (2.22) and (2.26), expressions describing microbial growth and substrate removal are:

$$\frac{dX}{dt} = \hat{\mu}\frac{SX}{K_S + S} \tag{2.28}$$

and

$$\frac{dS}{dt} = -k_m\frac{SX}{K_S + S} \tag{2.29}$$

k_m in equation (2.29) can also be written in terms of maximum specific substrate removal rate as follows:

$$k_m = \frac{\hat{\mu}}{Y} \tag{2.30}$$

Combining equations (2.28) and (2.30), specific substrate removal rate can be described with the following Monod-like expression:

$$q = k_m \frac{S}{K_S + S} \tag{2.31}$$

2.3.2 Microbial Decay

The endogenous decay rate is the rate of cell mass decrease per unit of mass, per time during endogenous respiration. Mathematically, microbial decay is defined by a first order rate expression with respect to the biomass concentration (Tchobanoglous & Burton, 2003):

$$\frac{dX}{dt} = -k_d X \tag{2.31}$$

2.3.3 Interpretation of Monod Equation

Values of $\hat{\mu}$ and K_S determine the relationship between substrate concentration, S and specific growth rate, μ. The four curves given in Figure 2.3 covers majority of domestic wastewaters (Orhon & Artan, 1994).

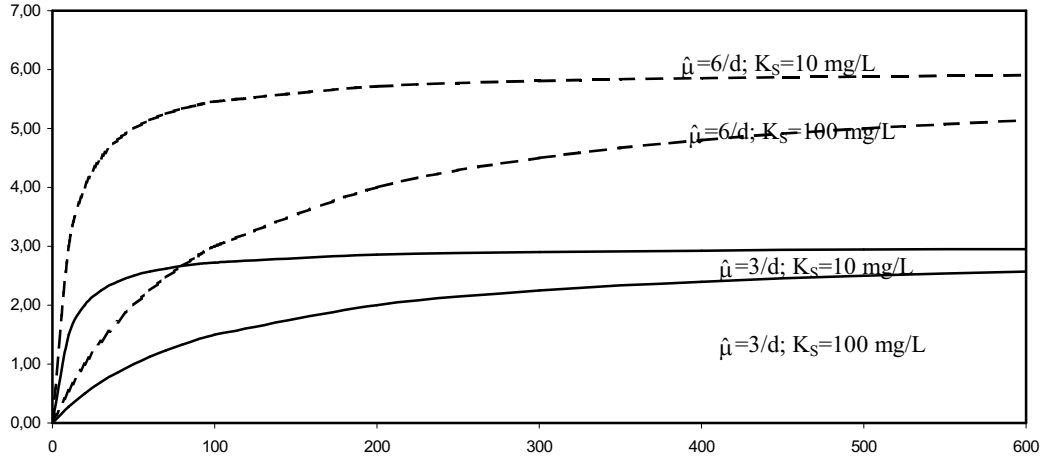

Figure 2.3 Effect of $\hat{\mu}$ and K_S over Monod equation

2.4 Method of Model Presentation

The mathematical models proposed to simulate the activated sludge system behavior involve a large number of reactions between a great number of components under various processes that occur in the system boundary. For a clear and definite representation of the systems and understanding of the models, the matrix format for the presentation of the activated sludge biokinetic model developed by Grady et al (1986) is used.

To illustrate the procedure for using the matrix format and notation, carbon removal by heterotrophic biomass under aerobic conditions is considered. In this situation, being general in activated sludge systems, the biomass increase and decay is the two fundamental processes that govern this system behavior. An example matrix describing this system, representing two fundamental processes is shown in Table 2.1.

Table 2.1 Matrix representation for biomass growth and decay (Henze at al, 1987)

Components →	i	1	2	3	Process Rate, ρ_j
j	Processes ↓	X_H	S	S_O	$[ML^{-3}T^{-1}]$
1	Growth	1	$-\frac{1}{Y_H}$	$-\left(\frac{1-Y_H}{Y_H}\right)$	$\hat{\mu}_H \frac{S}{K_S+S} X_H$
2	Decay	-1		-1	$k_d X_H$
Observed conversion rates $[ML^{-3}T^{-1}]$		$r_j = \sum_j r_{ij} = \sum_j \nu_{ij}\rho_j$			
Parameters $[ML^{-3}]$		Cell COD	COD	O_2 (-COD)	

It's required to identify the relevant system components in order to develop a matrix representation of the model. In this case, as mentioned above, three components are considered; biomass, substrate and dissolved oxygen, which are listed at the first row of the Table 2.1. The notation attributed system components is formed as follows: the insoluble constituents are given the symbol X and the soluble components S. Corresponding subscripts are attached to differentiate each

components as follows: H for heterotrophic biomass, S for substrate and S_O for oxygen. The index i ranging from 1 to 3 is assigned to each different component (Henze at al., 1987).

The next step is to define the biological processes occurring in the system. In this case, the biomass growth and decay are assumed to affect the concentration of the components in the system. These processes are listed in the first column of the Table 2.1. The index j, ranging from 1 to 2, refers to each process.

The kinetic expressions associated with the reactions occurring within system are placed at the last column of the Table 2.1. Here, process rates are denoted by ρ and the subscript, $_j$ in ρ_j is to indicate the j^{th} process in the matrix.

The stoichiometric coefficients are referred by the ν_{ij} notation to relate the action of j^{th} process upon the i^{th} components in the matrix. These coefficients are determined from mass balance relationships between components in each process. To illustrate, growth of biomass (+1) occurs at the expense of soluble substrate (-1/Y). In order to be consistent in terms of units, all coefficients and parameters are expressed in chemical oxygen demand (COD). The negative sign used in the matrix is to mean consumption and the positive sign is to refer to production (Henze at al., 1987).

The system reaction rate is the sum of all reaction rates corresponding to different processes occurring in the system.

$$r_{ij} = \nu_{ij}\rho_j \tag{2.32}$$

For example, the reaction rate regarding biomass, X_B, for growth and decay, as it is read from the matrix, would be:

$$r_j = \sum_j r_{ij} = \sum_j \nu_{ij}\rho_j \tag{2.33}$$

For soluble substrate, S, considering substrate utilization for biomass growth in the system, would be:

$$r_1 = r_{XH} = \hat{\mu}_H \frac{S}{K_S + S} X_H - k_d X_H \tag{2.34}$$

$$r_2 = r_S = -\frac{1}{Y_H} \hat{\mu}_H \frac{S}{K_S + S} X_H \tag{2.35}$$

$$r_3 = r_{SO} = -\frac{(1 - Y_H)}{Y_H} \hat{\mu}_H \frac{S}{K_S + S} X_H - k_d X_H \tag{2.36}$$

CHAPTER THREE
MATERIALS AND METHODS

In 1983, the International Association on Water Quality (IAWQ, formerly IAWPRC) formed a task group, which was to promote development, and facilitate the application of, practical models for design and operation of biological wastewater treatment systems. The first goal was to review existing models and the second goal was to reach a consensus concerning the simplest mathematical model having the capability of realistically predicting the performance of single-sludge systems carrying out carbon oxidation, nitrification and denitrification (Jeppsson, 1996). The final result was presented in 1987 (Henze et al., 1987) as the IAWQ Activated Sludge Model No.1.

Although the model has been extended since then, for example to incorporate more fractions of COD to accommodate new experimental observations (Sollfrank & Gujer, 1991), to describe growth and population dynamics of floc forming and filamentous bacteria (Kappeler & Gujer, 1992) and to include new processes for describing enhanced biological phosphorus removal (Henze et al., 1995), the original model is probably still the most widely used for describing WWT processes all over the world.

Due to the major impact of ASM1 on the WWT community it is considered as a 'state-of-the-art' model when biological phosphorus removal is not considered (Jeppsson, 1996). Monod relationship is used to describe the growth rate of both heterotrophic and autotrophic organisms. Unlike most of the previous models, COD was selected as the suitable parameter for defining the carbonaceous material, as it provides a link between electron equivalents in the organic substrate, the biomass and the oxygen utilized. Furthermore, mass balances can be made in terms of COD (Orhon & Artan, 1994).

Task group also introduced the concept of switching functions to gradually turn process rate equations on and off as the environmental conditions were changed. The switching functions are 'Monod-like' expressions that are mathematically continuous

and thereby reduce the problems of numerical instability during simulations (Jeppsson, 1996). The task group also presented the structure of biokinetic models in a matrix format described in previous chapter, which was easy to read and understand.

3.1 ASM1 Model Components

COD and nitrogen fractions are called as model components in the ASM1 model. COD and nitrogen fractions incorporated in ASM1 are discussed in following two sections.

3.1.1 Carbonaceous Components

COD is selected as the most suitable parameter for defining the carbon substrates as it provides a link between electron equivalents in the organic substrate, the biomass and oxygen utilized. In ASM1 the COD is subdivided based on solubility, biodegradability, biodegradation rate (Petersen, 2000):

- The total COD is divided into soluble (S) and particulate (X) components.

- The COD is further divided into non-biodegradable and biodegradable organic matter. The non-biodegradable matter is biologically inert and passes through an activated sludge system without any changes. The inert soluble organic matter (S_I) leaves the system at the same concentration as it enters. Inert suspended organic matter in the wastewater influent (X_I) or produced via decay (X_P) becomes enmeshed in the activated sludge and is removed from the system via the sludge wastage.

- The biodegradable matter is divided into soluble readily biodegradable (S_S) and slowly biodegradable (X_S) substrate. The readily biodegradable substrate is assumed to consist of relatively simple molecules that may be consumed directly by heterotrophic organisms and used for growth of new biomass. On

the contrary, the slowly biodegradable substrate consists of relatively complex molecules that require enzymatic breakdown prior to utilization.

- Finally, heterotrophic biomass (X_{BH}) and autotrophic biomass (X_{BA}) are generated by growth on the readily biodegradable substrate (S_S) or by growth on ammonia nitrogen (S_{NH}). The biomass is lost via the decay process and converted to X_P and X_S.

Figure 3.1 summarizes carbonaceous components incorporated in ASM1.

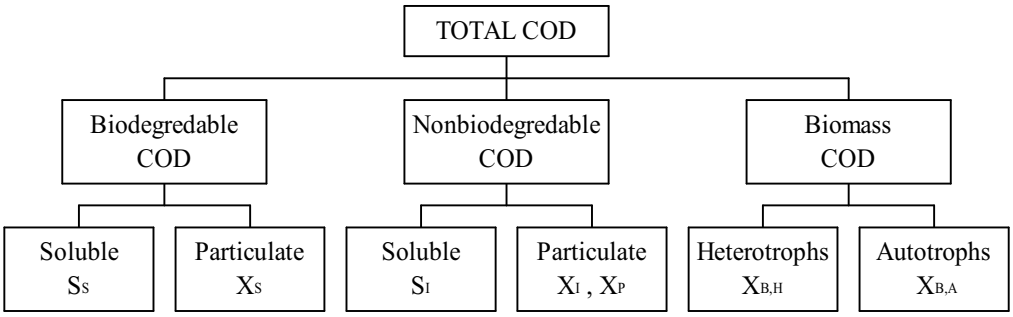

Figure 3.1 Carbonaceous components in ASM - 1

3.1.2 Nitrogenous Components

Similar to the organic matter, total nitrogen can be subdivided based on solubility, biodegradability and biodegradation rate (Petersen, 2000):

- Total nitrogen can be subdivided into soluble (S) and particulate (X) components.

- The nitrogen is divided into non-biodegradable matter and biodegradable matter. The non-biodegradable particulate organic nitrogen is associated with the non-biodegradable particulate COD (X_I or X_P), and the soluble non-biodegradable organic nitrogen is assumed to be negligible and not incorporated into the model.

- The biodegradable nitrogen is further divided into ammonia nitrogen (S_{NH}), nitrate + nitrite nitrogen (S_{NO}), soluble organic nitrogen (S_{ND}) and particulate organic nitrogen (X_{ND}). The particulate organic nitrogen is hydrolyzed to soluble organic nitrogen in parallel with hydrolysis of the slowly biodegradable organic matter (X_S). The soluble organic nitrogen is converted to ammonia nitrogen by ammonification. Ammonia nitrogen is the nitrogen source for biomass growth. Finally, the autotrophic conversion of ammonia results in nitrate nitrogen (S_{NO}), which is considered to be a single step process in ASM1.

Nitrogenous components in ASM1 are summarized in Figure 3.2.

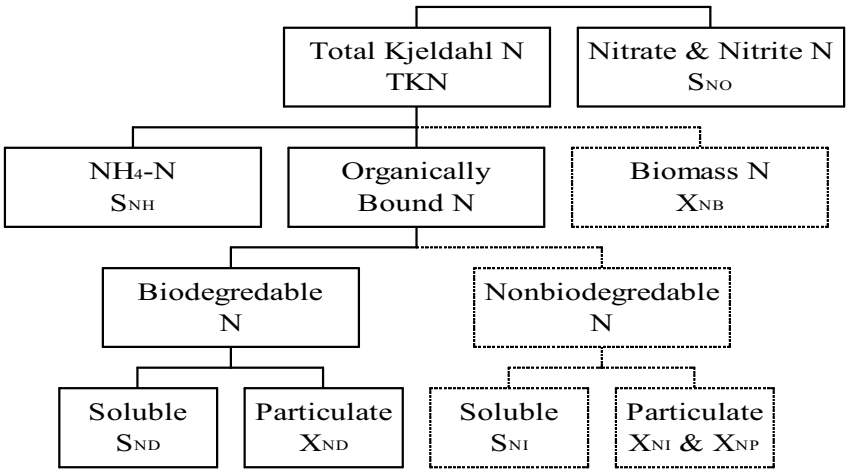

Figure 3.2 Nitrogenous components in ASM1. (Components shown in dotted frames are not included in the model although they can be calculated except S_{NI})

3.2 Model Processes

There are four different main processes defined in ASM1:

- Growth of biomass
- Decay of biomass
- Ammonification of organic nitrogen
- Hydrolysis of particulate organic matter

3.2.1 Aerobic Growth Of Heterotrophic Biomass

Growth occurs by degradation of soluble readily biodegradable substrate (S_S) and consumption of oxygen (S_O). Ammonia nitrogen (S_{NH}) is also incorporated into cell mass. Both the concentrations of S_S and S_O are rate limiting for the growth process. The Monod relationship is used to describe the growth of heterotrophic and autotrophic organisms (Henze et al., 1987).

3.2.2 Anoxic Growth Of Heterotrophic Biomass (Denitrification)

Heterotrophic organisms are capable of using nitrate as the terminal electron acceptor with S_S as substrate resulting in biomass growth and nitrogen gas in the absence of oxygen. Monod kinetics used for aerobic growth is applied except that the kinetic rate expression is multiplied by a correction factor ηg (<1). This factor is accounting for the fact that the anoxic substrate removal rate is slower compared to aerobic conditions. This can either be caused by a lower maximum growth rate or because only a fraction of the heterotrophic biomass is able to denitrify. (Sin, 2004) Furthermore, anoxic growth is inhibited when oxygen is present which is described by the switching function

$$\frac{K_{OH}}{K_{OH} + S_O} \tag{3.1}$$

The coefficient K_{OH} has the same value as in the expression for aerobic growth. Thus, as aerobic growth declines, the capacity for anoxic growth increases (Henze et al., 1987).

3.2.3 Aerobic Growth Of Autotrophic Biomass (Nitrification)

Ammonia nitrogen (S_{NH}) is oxidized to nitrate resulting in production of autotrophic biomass. A part of the S_{NH} is also incorporated in the autotrophic cell mass. As for heterotrophic growth the concentrations of S_{NH} and S_O can be rate

limiting for the process. Nitrification has a considerable effect on the alkalinity (S_{ALK}) (Henze et al., 1987).

3.2.4 Decay Of Heterotrophic Biomass

The death regeneration concept of Dold (1980) is applied to describe the different reactions that take place when organisms die. The traditional endogenous respiration concept describes how a fraction of the organism mass disappears to provide energy for maintenance. However, in the death regeneration concept oxygen is not directly associated with microbial decay. Decay is assumed to result in the release of slowly biodegradable substrate that is recycled back to soluble substrate and used for more cell growth. Thus, the oxygen utilization normally associated directly with decay is calculated as if it occurs indirectly from growth of new biomass on released substrate (Grady, 1999). A parallel conversion of organic nitrogen to ammonia nitrogen occurs. It should be noted that the magnitude of the decay coefficient used in this approach is different from that of the endogenous respiration (Orhon, 1994). In endogenous respiration the loss of one unit of biomass COD leads to the utilization of one unit of oxygen minus the COD of the inert particulate products that are formed. However, in the death regeneration model the loss of one biomass COD unit results in the ultimate formation of one unit of COD due to the formed readily biodegradable substrate minus the formed inert particulate products. When the readily biodegradable COD is used for cell synthesis, only a fraction of a unit of oxygen (determined by the yield) will be required because of the energy incorporated into the cell mass. That cell mass undergoes in turn decay etc. before the unit of oxygen is finally removed (Petersen, 2000).

As a summary, to give the same amount of oxygen utilization per time due to the decay process, the decay rate coefficient must be larger for the death regeneration concept than if a more traditional endogenous decay process was adopted (Orhon & Artan, 1994, Grady, *et al.*, 1999).

3.2.5 Decay Of Autotrophic Biomass

The decay of autotrophs is described similar to the heterotrophic decay process.

3.2.6 Ammonification Of Soluble Organic Nitrogen (S_{ND})

Biodegradable soluble organic nitrogen (S_{ND}) is converted to ammonia nitrogen (S_{NH}) in a first order process.

3.2.7 Hydrolysis

Slowly biodegradable substrate (X_S) in the sludge is broken down producing readily biodegradable substrate (S_S). The degradation of slowly biodegradable matter has appeared rather important to realistic modeling of activated sludge systems because it is primarily responsible for realistic electron acceptor profiles (Dold, 1980). This process is modeled on the basis of surface reaction kinetics and occurs only under aerobic and anoxic conditions. The hydrolysis rate is reduced under anoxic conditions in the same way as anoxic growth, by applying a correction factor ηh (<1) (Henze et al., 1987).

3.3 Model Formulation

Based on the component and processes described in previous two sections, ASM1 model can be formulated as ordinary differential equations. The equations are arranged in the matrix format described in section two by the task group is given in Table 3.1.

Table 3.1 ASM1 Model Matrix (Modified from Henze et al., 1987)

Component i	1	2	3	4	5	6	7	8	9	10	11	12	13	Process Rate, ρ_j $[ML^{-3}T^{-1}]$
j Process	S_I	S_S	X_I	X_S	$X_{B,H}$	$X_{B,A}$	X_P	S_O	S_{NO}	S_{NH}	S_{ND}	X_{ND}	S_{ALK}	
1 Aerobic growth of heterotrophs		$-\frac{1}{Y_H}$			1			$-\frac{1-Y_H}{Y_H}$		$-i_{XB}$			$-\frac{i_{XB}}{14}$	$\hat{\mu}_H\left(\frac{S_S}{K_S+S_S}\right)\left(\frac{S_O}{K_{O,H}+S_O}\right)X_{B,H}$
2 Anoxic growth of heterotrophs		$-\frac{1}{Y_H}$			1				$-\frac{1-Y_H}{2.86Y_H}$	$-i_{XB}$			$\frac{1-Y_H}{14x2.86Y_H}-\frac{i_{XB}}{14}$	$\hat{\mu}_H\left(\frac{S_S}{K_S+S_S}\right)\left(\frac{K_{O,H}}{K_{O,H}+S_O}\right)\left(\frac{S_{NO}}{K_{NO}+S_{NO}}\right)\eta_g X_{B,H}$
3 Aerobic growth of autotrophs						1		$-\frac{4.57-Y_A}{Y_A}$	$\frac{1}{Y_A}$	$-i_{XB}-\frac{1}{Y_A}$			$-\frac{i_{XB}}{14}-\frac{1}{7Y_A}$	$\hat{\mu}_A\left(\frac{S_{NH}}{K_{NH}+S_{NH}}\right)\left(\frac{S_O}{K_{O,A}+S_O}\right)X_{B,A}$
4 Decay of heterotrophs				$1-f_p$	-1		f_p					$-i_{XB}-f_p i_{XP}$		$b_H X_{B,H}$
5 Decay of autotrophs				$1-f_p$		-1	f_p					$-i_{XB}-f_p i_{XP}$		$b_A X_{B,A}$
6 Ammonification of soluble organic nitrogen										1	-1			$k_a S_{ND} X_{B,H}$
7 Hydrolisis of entrapped organics		1		-1										$k_H\frac{X_S/X_{B,H}}{K_X+X_S/X_{B,H}}\left[\left(\frac{S_O}{K_{O,H}+S_O}\right)+\eta_h\left(\frac{K_{O,H}}{K_{O,H}+S_O}\right)\left(\frac{S_{NO}}{K_{NO}+S_{NO}}\right)\right]X_{B,H}$
8 Hydrolisis of entrapped organic nitrogen											1	-1		$\rho_T(X_{ND}/X_S)$
Observed conversion rates $[ML^{-3}T^{-1}]$	$r_j=\sum_j \nu_{ij}\rho_j$													

In the following section, each model equation is written explicitly, in order to demonstrate how model components are affected by the processes.

Inert soluble organics (S_I) is not affected by any of eight processes included in ASM1 and therefore leaves the system at the same concentration as it enters. This component is included in the model only for simulation purposes.

The concentration of readily biodegradable substrate (S_S) is reduced by the growth of heterotrophic bacteria in both aerobic and anoxic conditions and is increased by hydrolysis of slowly biodegradable substrate. The differential equation describing this is:

$$\frac{dS_S}{dt} = \left[-\frac{\hat{\mu}_H}{Y_H}\left(\frac{S_S}{K_S + S_S}\right)\left\{\left(\frac{S_O}{K_{O,H} + S_O}\right) + \eta_g\left(\frac{K_{O,H}}{K_{O,H} + S_O}\right)\left(\frac{S_{NO}}{K_{NO} + S_{NO}}\right)\right\} + k_h \frac{X_S / K_{B,H}}{K_X + (X_S / X_{B,H})}\left\{\left(\frac{S_O}{K_{O,H} + S_O}\right) + \eta_h\left(\frac{K_{O,H}}{K_{O,H} + S_O}\right)\left(\frac{S_{NO}}{K_{NO} + S_{NO}}\right)\right\}\right] X_{B,H} \tag{3.2}$$

Inert suspended organic matter (X_I) becomes enmeshed in the activated sludge and is removed from the system via the sludge wastage. Like S_I, this component is also included in the model for simulation purposes.

The concentration of slowly biodegradable substrate (X_S) is increased by recycling of dead biomass according to the death-regeneration hypothesis and decreased by the hydrolysis process according to:

$$\frac{dX_S}{dt} = (1 - f_P)(b_H X_{B,H} + b_A X_{B,A}) -$$

$$k_h \frac{X_S / K_{B,H}}{K_X + (X_S / X_{B,H})} \left\{ \left(\frac{S_O}{K_{O,H} + S_O} \right) + \right. \tag{3.3}$$

$$\left. \eta_h \left(\frac{K_{O,H}}{K_{O,H} + S_O} \right) \left(\frac{S_{NO}}{K_{NO} + S_{NO}} \right) \right\} X_{B,H}$$

The dynamic behavior of the heterotrophic biomass ($X_{B,H}$) concentration is affected by aerobic and anoxic growth and decay of heterotrophs according to the following equation

$$\frac{dX_{B,H}}{dt} = \left[- \hat{\mu}_H \left(\frac{S_S}{K_S + S_S} \right) \left\{ \left(\frac{S_O}{K_{O,H} + S_O} \right) + \right. \right.$$

$$\left. \left. \eta_g \left(\frac{K_{O,H}}{K_{O,H} + S_O} \right) \left(\frac{S_{NO}}{K_{NO} + S_{NO}} \right) \right\} - b_H \right] X_{B,H} \tag{3.4}$$

For autotrophic biomass, the differential equation is simpler since autotrophs do not grow in anoxic environment. Concentration of autotrophic biomass is affected by anoxic growth and decay processes as follows:

$$\frac{dX_{B,A}}{dt} = \left[\hat{\mu}_A \left(\frac{S_{NH}}{K_{NH} + S_{NH}} \right) \left(\frac{S_O}{K_{O,A} + S_O} \right) - b_A \right] X_{B,A} \tag{3.5}$$

Like X_I, particulate inert organic products (X_P) arising from biomass decay also becomes enmeshed in the activated sludge and is removed from the system via the sludge wastage. The model equation describing X_P production is:

$$\frac{dX_P}{dt} = f_P (b_H X_{B,H} + b_A X_{B,A}) \tag{3.6}$$

The concentration of nitrate is affected by two processes. It's increased by nitrification and decreased by denitrification. Equation describing this is formulated below:

$$\frac{dS_{NO}}{dt} = -\hat{\mu}_H \eta_g \left(\frac{1-Y_H}{2.86Y_H}\right)\left(\frac{S_S}{K_S+S_S}\right)\left(\frac{K_{O,H}}{K_{O,H}+S_O}\right)\left(\frac{S_{NO}}{K_{NO}+S_{NO}}\right)X_{B,H} + \frac{\hat{\mu}_A}{Y_A}\left(\frac{S_{NH}}{K_{NH}+S_{NH}}\right)\left(\frac{S_O}{K_{O,A}+S_O}\right)X_{B,A} \tag{3.7}$$

The ammonia concentration is decreased by growth of all microorganisms as ammonia is used as the nitrogen source for incorporation into the biomass. The concentration is also decreased by the nitrification process and increased as a result of soluble organic nitrogen. The differential equation describing this is:

$$\frac{dS_{NH}}{dt} = \left[-i_{XB}\hat{\mu}_H\left(\frac{S_S}{K_S+S_S}\right)\left\{\left(\frac{S_O}{K_{O,H}+S_O}\right)+\eta_g\left(\frac{K_{O,H}}{K_{O,H}+S_O}\right)\left(\frac{S_{NO}}{K_{NO}+S_{NO}}\right)\right\}+k_a S_{ND}\right]X_{B,H} - \hat{\mu}_A\left(i_{XB}+\frac{1}{Y_A}\right)\left(\frac{S_{NH}}{K_{NH}+S_{NH}}\right)\left(\frac{S_O}{K_{O,A}+S_O}\right)X_{B,A} \tag{3.8}$$

The concentration of soluble organic nitrogen is increased by hydrolysis process and decreased by ammonification process according to:

$$\frac{dS_{ND}}{dt} = \left[-k_a S_{ND} + k_h \frac{X_{ND}/X_{B,H}}{K_X+(X_S/X_{B,H})}\left\{\left(\frac{S_O}{K_{O,H}+S_O}\right)+\eta_h\left(\frac{K_{O,H}}{K_{O,H}+S_O}\right)\left(\frac{S_{NO}}{K_{NO}+S_{NO}}\right)\right\}\right]X_{B,H} \tag{3.9}$$

The concentration of particulate organic nitrogen (X_{ND}) is increased by biomass decay and decreased by the hydrolysis process similar to the concentration of X_S. The differential equation describing this is:

$$\frac{dX_{ND}}{dt} = (i_{XB} - f_P i_{XP})(b_H X_{B,H} + b_A X_{B,A}) - k_h \frac{X_S / K_{B,H}}{K_X + (X_S / X_{B,H})} \left\{ \left(\frac{S_O}{K_{O,H} + S_O} \right) + \eta_h \left(\frac{K_{O,H}}{K_{O,H} + S_O} \right) \left(\frac{S_{NO}}{K_{NO} + S_{NO}} \right) \right\} X_{B,H} \tag{3.10}$$

The oxygen concentration in wastewater (S_O) is reduced by aerobic growth of heterotrophic and autotrophic microorganisms according to:

$$\frac{dS_O}{dt} = -\hat{\mu}_H \left(\frac{1 - Y_H}{Y_H} \right) \left(\frac{S_S}{K_S + S_S} \right) \left(\frac{S_O}{K_{O,H} + S_O} \right) X_{B,H} - \hat{\mu}_A \left(\frac{4.57 - Y_A}{Y_A} \right) \left(\frac{S_{NH}}{K_{NH} + S_{NH}} \right) \left(\frac{S_O}{K_{O,A} + S_O} \right) X_{B,A} \tag{3.11}$$

Finally, alkalinity (S_{ALK}) is increased by anoxic growth of heterotrophs (denitrification) and ammonification processes, and decreased by aerobic growth of both heterotrophs and autotrophs according to:

$$\frac{dS_{ALK}}{dt} = \left[\hat{\mu}_H \left(\frac{S_S}{K_S + S_S} \right) \left\{ -\frac{i_{XB}}{14} \left(\frac{S_O}{K_{O,H} + S_O} \right) + \eta_g \left(\frac{1 - Y_H}{14 x 2.86 Y_H} - \frac{i_{XB}}{14} \right) \left(\frac{K_{O,H}}{K_{O,H} + S_O} \right) \left(\frac{S_{NO}}{K_{NO} + S_{NO}} \right) \right\} + \frac{1}{14} k_a S_{ND} \right] X_{B,H} - \hat{\mu}_A \left(\frac{i_{XB}}{14} + \frac{1}{7 Y_A} \right) \left(\frac{S_{NH}}{K_{NH} + S_{NH}} \right) \left(\frac{S_O}{K_{O,A} + S_O} \right) X_{B,A} \tag{3.12}$$

3.4 Restrictions of ASM1

A number of restrictions concerning ASM1 are summarized below (Henze et al., 1987):

- The system must operate at constant temperature.

- The pH is constant and near neutrality. It is known that the pH has an influence on many of the parameters, however only limited knowledge is available to be able to express these possible influences. Consequently, a constant pH has been assumed. The inclusion of alkalinity in the model, however, does allow for detection of pH problems.

- No considerations have been given to changes in the nature of the organic matter within any given wastewater fractions (e.g. the readily biodegradable substrate). Therefore, the parameters in the rate expressions have been assumed to have constant values. This means that only concentration changes of the wastewater components can be handled whereas changes in the wastewater character cannot.

- The effects of nutrient limitations (e.g. N and P) on the cell growth have not been considered. It is, however, easy to add limitation terms in the model if needed.

- The correction factors for denitrification (ηg and ηh) are fixed and constant for a given wastewater, even though it is possible that their values are depending on the system configuration.

- The parameters for nitrification are assumed to be constant and to incorporate any inhibitory effects that wastewater constituents may have on them.

- The heterotrophic biomass is homogeneous and does not undergo changes in species diversity with time. This assumption is inherent to the assumption of constant kinetic parameters. This means that any changes in substrate concentration gradients, reactor configuration, etc. on sludge settleability are not considered.

- The entrapment of particulate organic matter in the biomass is assumed to be instantaneous.

- The hydrolysis of organic matter and organic nitrogen are coupled and occur simultaneously with equal rates.

- The type of electron acceptor present does not affect the loss of biomass by decay.

- The type of electron acceptor does not affect the heterotrophic yield coefficient.

- ASM1 is developed for simulation of treatment of municipal wastewater, and it is therefore not advised to apply the model to systems where industrial contributions dominate the characteristics of the wastewater.

- ASM1 cannot deal with elevated nitrite concentrations.

- ASM1 is not designed to deal with activated sludge systems with very high load or small sludge retention time (SRT<1 day).

3.5 Model Calibration Methods

Model calibration is adaptation of a model to fit a certain set of information obtained from the full-scale WWTP under study. This task is often time-consuming and typically the time needed for a model calibration is underestimated. Even though

more than a decade has passed since the publication of ASM1, a fully developed model calibration procedure has not been defined yet (Petersen, 2000).

There isn't a complete procedure for calibration of ASM1. There may be many reasons for this. Important to realize is that the purpose of a model being built is very much determining on how to approach the calibration, making it difficult to generalize (Henze et al., 1995). Usually model calibration procedures depend on the applications, e.g. for process scenarios and optimizations etc. To obtain information on model calibration procedures one often has to collect bits and pieces from various sources to obtain an overview (Petersen, 2000).

Parameter estimation consists of determining the optimal values of the parameters of a given model with the aid of measured data. Initially, the model structures, of which selected parameters need to be estimated, and the experimental data need to be defined. Moreover, first guesses of the initial conditions, i.e. concentrations, and parameters, have to be given (Petersen, 2000). The parameter estimation routine then basically consists of minimizing an objective function, which for example can be defined as the weighted sum of squared errors between the model output and the data (Fikar et al., 2002). When the objective function reaches a minimum with a certain given accuracy the optimal parameter values are obtained. Thus, parameter estimation is carried out using specific mathematical search algorithms.

However, due to the high complexity caused by the numerous parameters and the unidentifiable nature of the ASM models, it will be hard to apply mathematical calibration techniques. A major problem encountered in calibration of ASM is the identifiability of the model parameters (Petersen, 2000). Identifiability is the ability to obtain a unique combination of parameters describing system behavior. A distinction should be made between theoretical and practical identifiability. Theoretical identifiability is a property of the model structure, and relates to the question whether it is at all possible to obtain unique parameter values for a given model structure considering certain selected outputs, and assuming ideal measurements. Practical identifiability, on the other hand, includes the quality of the

data. Thus, theoretically identifiable parameters may be practically unidentifiable if the data are too noise corrupted (Jeppsson, 1996).

When estimating model parameters, it must always be noted that a typical problem related to the model calibration of ASM is that more than one combination of influent characteristics and model parameters can give the same good description of the collected data (Kristensen et al., 1998). This indicates identifiability problems of either theoretical or practical origin.

Regarding theoretical and practical identifiability problems of model parameters, model calibration of ASM is typically based on a step-wise procedure, and by changing just a few of the many parameters instead of applying an automatic mathematical optimization routine (Petersen, 2000).

3.5.1 Information Set For Model Calibration

The set of information that should be collected for successful model calibration was extracted and combined from different sources (Henze et al., 1987; Henze, 1992; Lesouef et al., 1992; Xu & Hultman, 1996; Kristensen et al., 1998, Petersen, 2000), and is summarized below:

- Design data: reactor volumes pump flows and aeration capacities.

- Operational data:
  - Flow rates, as averages or dynamic trajectories, of influent, effluent, recycle and waste flows.
  - pH, aeration and temperatures.

- Characterization for the hydraulic model, e.g. the results of tracer tests.

- Characterization for the settler model: e.g. zone settling velocities at different mixed liquor suspended solids concentrations.

- Characterization for the biological model, ASM, of:
    - Wastewater concentrations of full-scale WWTP influent and effluent (as well as some intermediate streams between the WWTP's unit processes), as averages or as dynamic trajectories: e.g. SS, COD, TKN, NH_4-N, NO_3-N, PO_4-P etc.
    - Sludge composition: e.g. SS, VSS, COD, N and/or P content.
    - Reaction kinetics: e.g. growth and decay rates.
    - Reaction Stoichiometry: e.g. biomass yields

The list does not describe how the particular information can be collected in practice. As mentioned above, the required quality and quantity of information will depend very much on the purpose of the modeling exercise. In case the model is to be used for educational purposes, for comparison of design alternatives for non-existing plants or in other situations where qualitative comparisons are sufficient, the default parameter values defined by Henze et al. (1987) can be applied (Petersen, 2000). A reasonably good description can most often be obtained with this default parameter set for typical municipal cases without significant industrial influences (Henze et al., 1997).

However, some processes may need a more adequate description than others depending on the purpose of the model calibration. This may especially apply for models that are supposed to describe the processes in an industrial or combined municipal and industrial treatment plant (Petersen, 2000). In such cases the wastewater characterization and the activated sludge may differ significantly from standard municipal wastewater. Also, the availability of readily biodegradable carbon substances is important for the successful achievement of both denitrification and biological P removal, and may need to be characterized in more detail (Petersen, 2000).

The information needed for the characterization of the biological model can basically be gathered from three sources (Petersen, 2000):

- Default values from literature (e.g. Henze et al., 1987).

- Full-scale plant data
  - Average or dynamic data from grab or time/flow proportional samples.
  - Conventional mass balances of the full-scale data.
  - On-line data.
  - Measurements in reactors to characterize process dynamics (mainly relevant for SBR's and alternating systems).
  - Information obtained from different kinds of lab-scale experiments with wastewater and activated sludge from the full-scale plant under study.

The intended use of the model will determine which information source to choose for the characterization of the different biological processes in the model. Furthermore, the purpose will decide to which level the model has to be calibrated, since the quality of the desired model predictions will depend strongly on the quality of the model calibration (Petersen, 2000).

3.5.2 Model Calibration Levels

3.5.2.1 Steady State Model Calibration

In this step, assuming that the average represents a steady state, data obtained from the full-scale WWTP are averaged and a simple model not including hydraulic detail is calibrated to average effluent and sludge waste data. Typically, the calibrations of the ASM and the settler are linked together, since the aim is most often to describe the final effluent quality. The recycle from the settler also has an influence on the activated sludge system. Thus, there may be an interaction between the steady state calibration and the settler model calibration. Finally, the

characterization of wastewater components may be adjusted according to the calibration of the full-scale model (Jeppsson, 1996).

The next step in the calibration procedure is a steady state model calibration that includes the hydraulic model. In general, with a steady state model calibration, only parameters responsible for long-term behavior of the WWTP can be determined, i.e. Y_H, f_p, b_H and X_I in the influent (Henze et al., 1999; Nowak et al., 1999). These parameters are correlated to a certain degree, meaning that a modification of one parameter value can be compensated by a modification of another parameter value. In the study of Nowak et al. (1999) on mass balances of full-scale data, it was therefore chosen to fix Y_H and f_p, leaving X_I in the influent and b_H to be determined from the steady state data. In the study of Lesouef et al. (1992), two WWTP models were calibrated via steady state calibration only, and this calibrated model was applied to simulate dynamic process scenarios. A steady state calibration is, very useful for the determination of initial conditions prior to a dynamic model calibration and for the initiation of first parameter iteration (Kristensen et al., 1998; Petersen, 2000).

3.5.2.2 *Dynamic Model Calibration*

If it is the aim to describe and predict more short-term and dynamic situations, a model calibration to dynamic data will be needed since such data contain more information than steady state data, especially on fast dynamic behavior. The important point in model calibration based on dynamic data is to obtain a more reliable estimation of the maximum specific growth rates μ_{maxH} and μ_{maxA} (Henze et al., 1999), which are the most important parameters in predicting dynamic situations.

At WWTP's data are most often collected routinely with a daily or weekly sampling frequency. This sampling frequency may, however, not be high enough, and for more accurate modeling it may therefore be required to run special measuring campaigns. The sampling frequencies should be chosen in relation to the time constants of the process and influent variations. One of the important time constants

of the process is the hydraulic retention time (HRT). Ideally, one should choose to sample about five times faster than the hydraulic retention time and have a test duration of 3-4 times this key time constant (Ljung, 1987). However, since measurements on full-scale WWTP's are relatively expensive these recommendations may not always be completely fulfilled. Furthermore, data from the full-scale installation alone may be insufficient for a dynamic model calibration since the reaction kinetics can not be readily obtained from such data, except for specific designs like SBR's and alternating systems (Petersen, 2000). For a dynamic model calibration on a full-scale WWTP the modeler is therefore typically aiming at combining more information rich results derived from lab-scale experiments (carried out with sludge and wastewater from the full-scale installation) with data obtained from measuring campaigns on the WWTP under study (Dupont and Sinkjær, 1994). In the studies of Dupont and Sinkjær (1994) the emphasis was to have a description of the nitrification and denitrification, and the model calibrations therefore focused on adjustment of the parameters related to these processes. In contrast, other studies aimed at a description of both COD and N removal, and as a result more parameters had to be considered for adjustment in the model calibration (Kristensen et al., 1998).

The wastewater characterization has both been carried out via full-scale data combined with mass balances and via lab-scale experiments, e.g. for the inert components S_I and X_I (Lesouef et al., 1992) and the S_S component (Kristensen et al., 1998). In one study all wastewater components were determined via calibration on the full-scale data (de la Sota et al., 1994). The determination of the stoichiometric and kinetic parameters is often carried out via calibration of the model to the full-scale data only (Petersen et al., 2000).

3.5.3 *Characterization of Wastewater*

Different methods are proposed to structure the wealth of methods that have been developed and applied for the characterization of wastewater and reaction kinetics in relation to ASM1.

Wastewater can be characterized either with physical-chemical methods or with biological methods. In practice one typically ends up with a combined approach to obtain an estimate of the concentrations of all components (Petersen et al., 2000). In ASM1 the COD_{tot} of the wastewater is considered to consist of inert soluble organic matter (S_I), readily and slowly biodegradable substrate (S_S and X_S respectively) and inert suspended organic matter (X_I), whereas biomass in the wastewater is considered to be insignificant.

A wastewater can be separated into different components in a relatively simple manner via physical-chemical separation methods. The difference in molecular size can give an indication on biodegradability because small molecules can be taken up directly over the cell membranes whereas bigger molecules need to be broken down prior to uptake (Sin, 2000). Enzymatic hydrolysis is primarily a surface phenomenon, which means that the hydrolysis rate is directly related to the surface area. Thus, smaller molecules are readily degraded whereas degradation of larger material can be kinetically limited (Grady et al., 1999).

The ASM models do not differentiate between filtered, colloidal and settleable wastewater fractions. It is therefore necessary to convert the fractions resulting from a physical-chemical characterization to the ASM components. The possibilities and limitations of physical-chemical methods to accomplish this task are summarized below.

3.5.3.1 Inert Soluble Organic Matter

Soluble inert organic matter (S_I) is present in the influent, but also produced during the activated sludge process (Orhon & Artan, 1994). Most of the evidence for the production of soluble organics by microorganisms is collected from experiments with simple known substrates, e.g. glucose (Petersen et al., 2000). However, the production has also been proven to take place with wastewater (Orhon & Artan, 1994). A model has been proposed relating the S_I formation to the hydrolysis of non-viable cellular materials in the system, thereby linking the S_I production to the initial

substrate concentration and the decay of the produced biomass (Orhon & Artan, 1994). This model was verified in a study with different industrial wastewaters and, although the data were not of very high quality, some evidence was given that the S_I production depends very much on the wastewater type (Petersen, 2000). Although the origin of the S_I production may remain unexplained, it seems clear that it does take place to various extents depending on different factors as mentioned above, resulting in a S_I concentration in the effluent that may be higher than the influent. Such S_I production is, however, not included in the ASM models, where S_I is considered a conservative component. To deal with this discrepancy between model concept and reality a simplified approach is typically applied by the definition of a fictive model influent concentration S_I that includes the produced S_I together with the real S_I influent concentration (Henze, 1992).

It is not possible to measure S_I directly and different approximations are therefore usually applied. Most often S_I is determined by the soluble effluent COD, which has appeared to be a good estimate for S_I in case of a low loaded activated sludge process (Ekama et al., 1986). On the other hand Siegrist and Tschui (1992) suggested that the influent S_I could be estimated as 90% of the effluent COD. These approximations may hold in most cases, but a more correct approach would be to consider it as the soluble effluent COD minus the soluble effluent Biochemical Oxygen Demand (BOD) multiplied with a BOD/COD conversion factor (Henze, 1992). Furthermore, S_I can be determined as the soluble COD remaining after a long-term BOD test with the influent (Henze et al., 1987). The latter approach is in fact a combination of physical-chemical and biological methods.

Summarizing, it will be case depending whether it is needed to characterize the produced S_I or whether the model component can be approximated as described above.

3.5.3.2 Readily Biodegradable Substrate

The soluble COD fraction excluding the soluble inert organic matter (S_I) is mostly considered to be the readily biodegradable substrate (S_S). The correctness of this approach does however evidently depend on the pore size of the filters used for the separation. It was confirmed biologically with respirometric methods, that the studied wastewater did not contain any particulate readily biodegradable matter (Petersen, 2000).

Finally, a method based on flocculation with $Zn(OH)_2$ has been developed to remove colloidal matter of 0.1-10 μm that normally passes through 0.45 μm filter membranes, and was successfully applied to a nitrifying (Sin, 2000) and phosphorus removal activated sludge system (Mamais et al., 1993, Petersen, 2000).

3.5.3.3 Inert Suspended Organic Matter

The test proposed for the determination of S_I, as the residual soluble COD remaining after a long-term BOD test, by Lesouef et al. (1992) can also be applied to determine X_I (Petersen et al., 2000). The X_I concentration is then determined as the residual particulate COD, assuming that X_I is not produced during the test. This assumption may, however, be questionable since X_I will be produced due to decay during the long-term BOD test and corrections for this will have to be considered. It is also proposed that X_I should be estimated by comparing the effective sludge production in the full-scale plant with simulation (Sin, 2000).

3.5.3.4 Slowly Biodegradable Substrate

A physical characterization based on different molecular sizes can be used to distinguish between readily biodegradable substrate S_S and slowly biodegradable substrate X_S (Petersen et al., 2000). If the components S_S, S_I and X_I are known and if it is assumed that the biomass concentration is negligible, X_S can be determined via a simple mass COD balance.

3.5.3.5 Biomass

It is not possible to determine biomass concentrations (X_{BH} *and* X_{BA}) with a physical-chemical method.

3.5.3.6 Nitrogen Components

The nitrogen components (S_{NH}, S_{ND}, S_{NO}, X_{ND}) can rather easily be detected by physical–chemical analysis via a combination of standard analyses of ammonium, nitrite and nitrate and Kjeldahl nitrogen (TKN) on filtered and nonfiltered samples (Henze et al., 1987).

CHAPTER FOUR
APPLICATIONS

4.1 Güneybatı Wastewater Treatment Plant

Güneybatı Wastewater Treatment Plant is located in the southwest region of İzmir treating domestic wastewaters of Güzelbahçe, Balçova and Narlıdere Municipalities. The plant also receives wastewater of the military school located nearby.

The plant is designed to treat 21600 m^3/ day of wastewater and consists of coarse and fine screens, aerated grit chamber, anaerobic mixing tank, chemical dosage system for phosphorus precipitation, aeration tanks, secondary clarifiers, coastal discharge system and mechanical sludge dewatering systems.

Wastewater inflow enters the plant passing through 50 mm coarse screens and 10 mm fine screens followed by 2 aerated grit chambers. Oil and grease is removed in these units together with grit. Residuals from these pretreatment units are then transferred to Harmandalı landfill.

After pretreatment, wastewater enters two anaerobic mixing tanks with a total volume of 2700 m^3 for biological excess phosphorus removal. Tanks are mixed under anaerobic conditions via 8 mixers. A chemical dosage system is also installed for chemical phosphorus precipitation.

The flow then passes to two aeration tanks with a total volume of 10042 m^3. Nitrification and denitrification processes occur in these tanks together with carbon oxidation. To maintain anoxic conditions in aeration tanks, only 65% of the tanks are aerated via 1560 diffusers. Air is supplied from 5 blowers each with a capacity of 2250 m^3/h.

In secondary clarifiers, biomass is separated form wastewater and treated wastewater then enters to the coastal discharge system. A portion of the resulting

sludge is pumped back to the anaerobic mixing tanks and waste sludge is pumped to sludge dewatering unit. Sludge is dewatered in this unit via belt-filters. Dewatered sludge is then transferred to Uzundere composting plant.

Finally, treated wastewater is discharged to İzmir Bay, passing through an HDPE discharge line with a diameter of 630 mm.

4.2 Single Sludge Simulation Program

Single Sludge Simulation Program (SSSP) was developed in 1988 by Bidstrup and Grady to simulate activated sludge processes by solving ASM1 model equations. Other most popular simulation programs developed to simulate activated sludge plants using ASM1 are AQUASIM (Reichert, 1994), GPSX (Hydromantis Inc.), STOAT (Arant, 1999) and EFOR (Kruger Systems, 1993).

SSSP is an interactive program that simulates activated sludge processes performing carbon oxidation, nitrification and denitrification in multiple completely mixed reactors arranged in series by using ASM1 model. SSSP is programmed in Borland's Turbo Pascal language.

```
                    MAIN MENU

 (1)  ENTER the title of the simulation.
 (2)  ENTER the kinetic and stoichiometric parameters.
 (3)  ENTER the steady-state feed composition.
 (4)  DEFINE the process flow scheme and operating parameters.
 (5)  SOLVE for the steady-state case.
 (6)  DISPLAY the errors and warnings file.
 (7)  DISPLAY the steady-state results.
 (8)  HARD COPY menu.
 (9)  FILE operations.
(10)  STORE process variables.
(11)  CURVE plotting routine.
(12)  HISTOGRAM plotting routine.
(13)  DYNAMIC solution menu.
(14)  QUIT and return to system command.

      Enter choice by number and press <return> ?

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```
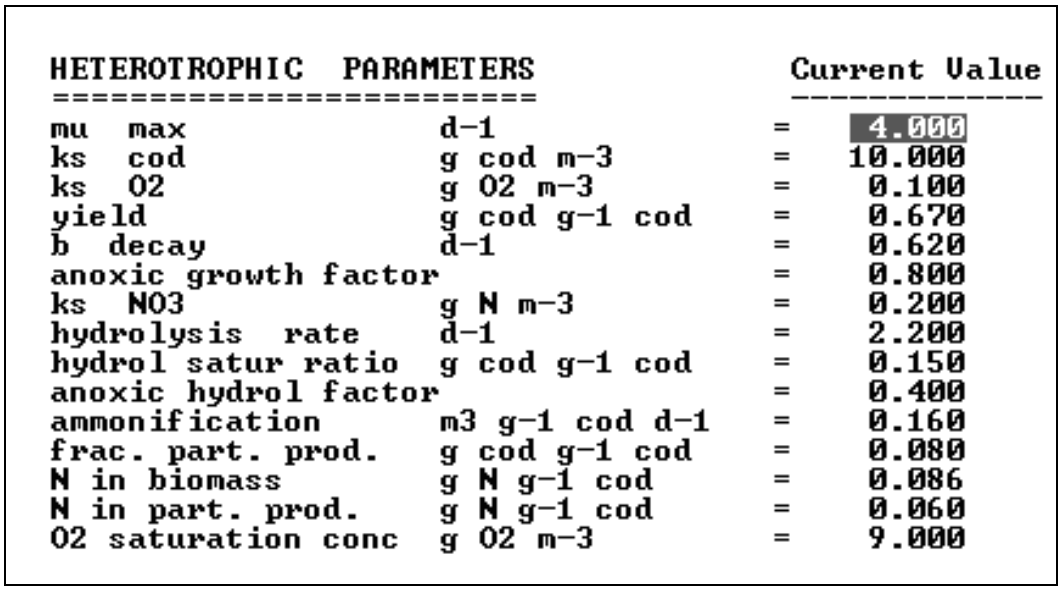

Figure 4.1 Main menu of SSSP

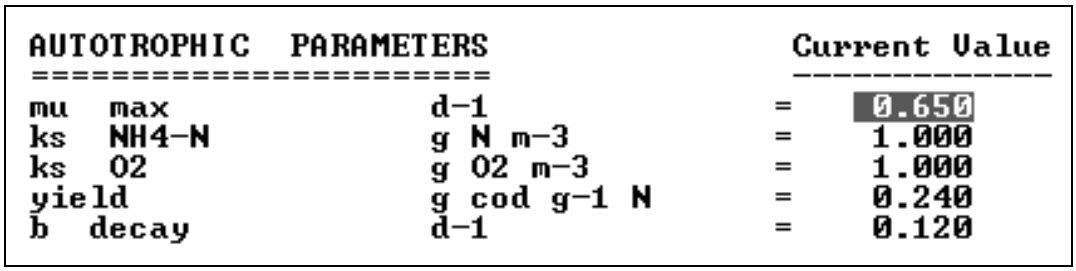
Main menu of SSSP is given in Figure 4.1. The first four options specify the system to be simulated. Through these options kinetic and stoichiometric parameters, feed wastewater composition as well as the hydraulic properties and process flow scheme of the system are designated. Options 5 and 13 are for steady-state and dynamic calculations respectively while the rest are options for controlling the program.



HETEROTROPHIC PARAMETERS			Current Value
mu max	d-1	=	4.000
ks cod	g cod m-3	=	10.000
ks O2	g O2 m-3	=	0.100
yield	g cod g-1 cod	=	0.670
b decay	d-1	=	0.620
anoxic growth factor		=	0.800
ks NO3	g N m-3	=	0.200
hydrolysis rate	d-1	=	2.200
hydrol satur ratio	g cod g-1 cod	=	0.150
anoxic hydrol factor		=	0.400
ammonification	m3 g-1 cod d-1	=	0.160
frac. part. prod.	g cod g-1 cod	=	0.080
N in biomass	g N g-1 cod	=	0.086
N in part. prod.	g N g-1 cod	=	0.060
O2 saturation conc	g O2 m-3	=	9.000

Figure 4.2 Default kinetic and stoichiometric parameters for heterotrophic biomass

SSSP menu for the kinetic and stoichiometric parameters for heterotrophic biomass is presented in Figure 4.2. Corresponding values for each parameter are default values offered by the IAWQ task group.



AUTOTROPHIC PARAMETERS			Current Value
mu max	d-1	=	0.650
ks NH4-N	g N m-3	=	1.000
ks O2	g O2 m-3	=	1.000
yield	g cod g-1 N	=	0.240
b decay	d-1	=	0.120

Figure 4.3 Default kinetic and stoichiometric parameters for autotrophic biomass

SSSP menu for the kinetic and stoichiometric parameters for autotrophic biomass is presented in Figure 4.3. Corresponding values for each parameter are default values offered by the IAWQ task group.

4.3 Calibration of ASM1

ASM1 model is calibrated with influent and effluent data obtained from plant between 01.07.2005 and 31.07.2005. Data obtained from the plant is given in Table 4.1 and removal efficiency of COD and Total Kjeldahl Nitrogen is given in Table 4.2. COD and nitrogen is fractionated using the proposed percentages by IWA Task Group (Henze et al., 1987).

4.3.1 COD and Nitrogen Fractions

Literature data on COD fractionation from different authors are collected from different authors are summarized in Table 4.2. As discussed in previous chapter, COD fractionation is determined on a long-term (average) basis. In absence of physical-chemical and respirometric tests, soluble inert organic matter concentration may be calculated by considering it as effluent COD minus the effluent Biochemical Oxygen Demand (BOD) multiplied with a BOD/COD conversion factor (Henze, 1992). Inert suspended organic matter, on the other hand, should be evaluated by entering remaining parameters to the simulation (Henze, 1992; Sin, 2000).

Table 4.1. Influent and effluent COD and TKN concentrations

Date	Influent			Operating Parameters			Effluent	
	Flowrate	COD	TKN	MLSS	Sludge Recycle	Sludge Wastage	COD	TKN
	m3/d	Mg/L	mg/L	mg/L	m3/d	kg SS/d	mg/L	mg/L
01.07.2005	16202,0	361,5	14,8	4140,0	21600,0	4285,0	46,8	2,5
02.07.2005	16717,0	-(*)	-	-	21600,0	-	-	-
03.07.2005	12292,0	-	-	-	21600,0	-	-	-
04.07.2005	18019,0	300,3	16,5	2340,0	21600,0	3511,0	58,8	5,9
05.07.2005	15372,0	293,8	14,3	2060,0	10800,0	2654,0	57,7	4,6
06.07.2005	14783,0	481,9	16,3	1500,0	10800,0	104,0	61,6	8,0
07.07.2005	16062,0	327,0	15,3	1000,0	13200,0	0,1	85,9	11,9
08.07.2005	16366,0	303,4	15,8	5100,0	13200,0	3387,0	75,7	10,8
09.07.2005	16333,0	322,0	15,8	4760,0	13200,0	5589,0	71,6	9,5

Continued from Table 4.1

10.07.2005	14720,0	-	-	-	13200,0	-	-	-
11.07.2005	15520,0	241,1	14,1	3800,0	13200,0	3355,0	61,2	1,4
12.07.2005	16479,0	326,4	15,0	3620,0	13200,0	3441,0	57,6	3,4
13.07.2005	17213,0	305,4	15,8	3080,0	13200,0	3557,0	61,6	4,4
14.07.2005	18074,0	251,7	15,1	2500,0	13200,0	2688,0	53,0	5,9
15.07.2005	18063,0	205,7	15,3	3100,0	13200,0	4818,0	71,7	8,8
16.07.2005	17645,0	-	-	-	13200,0	-	-	-
17.07.2005	16542,0	-	-	-	10800,0	-	-	-
18.07.2005	16253,0	347,6	15,7	3460,0	10800,0	5071,0	71,2	11,3
19.07.2005	15423,0	202,7	16,5	3020,0	10800,0	3142,0	132,3	9,6
20.07.2005	16400,0	436,8	47,3	1620,0	21600,0	0,0	66,2	10,7
21.07.2005	17016,0	293,7	17,2	3360,0	21600,0	1481,0	71,1	13,4
22.07.2005	16770,0	262,0	16,5	5820,0	21600,0	2358,0	70,4	11,3
23.07.2005	16897,0	-	-	-	21600,0	-	-	-
24.07.2005	15564,0	-	-	-	21600,0	-	-	-
25.07.2005	16602,0	182,1	15,2	2940,0	21600,0	4257,0	98,3	10,9
26.07.2005	16850,0	310,4	22,0	3440,0	21600,0	4111,0	72,9	6,4
27.07.2005	16694,0	204,2	14,7	2980,0	21600,0	3191,0	76,2	7,9
28.07.2005	16637,0	206,4	7,7	2860,0	21600,0	2397,0	68,8	7,7
29.07.2005	16879,0	160,0	14,0	2300,0	21600,0	2533,0	64,0	1,9
30.07.2005	16618,0	-	-	-	21600,0	-	-	-
31.07.2005	16443,0	-	-	-	21600,0	-	-	-
Average	16369,0	278,5	16,9	3127,0	17148,0	2747,0	70,7	7,6

*** -:** Not measured

The nitrogen components *(S_{NH}, S_{ND}, S_{NO}, X_{ND})* can rather easily be detected by physical–chemical analysis via a combination of standard analyses of ammonium, nitrite and nitrate and Kjeldahl nitrogen (TKN) (Henze et al., 1987). Literature data on N Fractionation is summarized in Table 4.3.

Table 4.2 Comparison of different literature data on COD fractions

	Henze et al (1987)	Kappeler & Gujer (1992)	Sollfrank (1988)	Park et al (1997)	Ekama et al (1986)
S_S	25 %	9 %	16 %	30 %	10 – 35 %
S_I	10 %	11 %	10 %	7 %	5 – 20 %
X_S	45 %	58 %	40 %	48 %	-
X_H	-	12 %	25 %	-	-
X_I	15 %	10 %	25 %	15 %	2 – 3 %

-: Not Available

Table 4.3 Comparison of different literature data on N fractions

	Henze et al(1987)	Fikar et al (2002)
S_{NH}	63 %	66 %
S_{ND}	16 %	2 %
S_{NO}	0 %	0 %
X_{ND}	21%	32 %

Task group's proposed COD and N fractionation is widely used in recent studies in absence of experimental data. These data are used in model calibration except for S_I and results obtained are shown in Table 4.4. COD and N fractions used in calibration study are summarized in table 4.5.

Table 4.4 COD and N Fractionation

	Concentration mg/L	Percentage
S_S	69.6	25 %
S_I	62.5	23 %
X_S	125.3	45 %
X_H	0.0	0 %
X_I	21.1	7 %
S_{NH}	10.6	63 %
S_{ND}	2.7	16 %
S_{NO}	0	0 %
X_{ND}	3.5	21 %

Table 4.5 Calculated COD and N fractions

Date	Carbonecious Components					Nitrogenious Compounds			
	mg COD/L					mg N/L			
	Total	SI	SS	XI	XS	TKN	SNH	SND	XND
01.07.2005	361,5	83,1	90,4	25,3	162,7	14,8	9,3	2,4	3,1
04.07.2005	300,3	69,1	75,1	21,0	135,1	16,5	10,4	2,6	3,5
05.07.2005	293,8	67,6	73,5	20,6	132,2	14,3	9,0	2,3	3,0
06.07.2005	481,9	110,8	120,5	33,7	216,9	16,3	10,3	2,6	3,4
07.07.2005	327,0	75,2	81,8	22,9	147,2	15,3	9,6	2,4	3,2
08.07.2005	303,4	69,8	75,9	21,2	136,5	15,8	10,0	2,5	3,3
09.07.2005	322,0	74,1	80,5	22,5	144,9	15,8	10,0	2,5	3,3
11.07.2005	241,1	55,5	60,3	16,9	108,5	14,1	8,9	2,3	3,0
12.07.2005	326,4	75,1	81,6	22,8	146,9	15,0	9,5	2,4	3,2
13.07.2005	305,4	70,2	76,4	21,4	137,4	15,8	10,0	2,5	3,3
14.07.2005	251,7	57,9	62,9	17,6	113,3	15,1	9,5	2,4	3,2
15.07.2005	205,7	47,3	51,4	14,4	92,6	15,3	9,6	2,4	3,2
18.07.2005	347,6	79,9	86,9	24,3	156,4	15,7	9,9	2,5	3,3
19.07.2005	202,7	46,6	50,7	14,2	91,2	16,5	10,4	2,6	3,5
20.07.2005	436,8	100,5	109,2	30,6	196,6	47,3	29,8	7,6	9,9
21.07.2005	293,7	67,6	73,4	20,6	132,2	17,2	10,8	2,8	3,6
22.07.2005	262,0	60,3	65,5	18,3	117,9	16,5	10,4	2,6	3,5
25.07.2005	182,1	41,9	45,5	12,7	81,9	15,2	9,6	2,4	3,2
26.07.2005	310,4	71,4	77,6	21,7	139,7	22,0	13,9	3,5	4,6
27.07.2005	204,2	47,0	51,1	14,3	91,9	14,7	9,3	2,4	3,1
28.07.2005	206,4	47,5	51,6	14,4	92,9	7,7	4,9	1,2	1,6
29.07.2005	160,0	36,8	40,0	11,2	72,0	14,0	8,8	2,2	2,9
Average	278,5	64,1	69,6	19,5	125,3	16,9	10,6	2,7	3,5

4.3.2 Kinetic and Stoichiometric Coefficients

Default kinetic and stoichiometric parameters proposed the by task group are used in model calibration.

CHAPTER FIVE
RESULTS AND DISCUSSION

5.1 Simulation Studies

A steady-state simulation application is performed on the basis of above data. Simulated result for effluent COD compared with measured actual plant data is presented in Figure 5.1. Simulation results for COD removal are presented in Table 5.1.

Table 5.1 Influent, measured and simulated COD concentrations

Date	Influent mg/L	Effluent Measured mg/L	Effluent Simulated mg/L
01.07.2005	361.5	46.8	88.0
04.07.2005	300.3	58.8	74.0
05.07.2005	293.8	57.7	72.4
06.07.2005	481.9	61.6	115.3
07.07.2005	327.0	85.9	80.0
08.07.2005	303.4	75.7	74.6
09.07.2005	322.0	71.6	78.9
11.07.2005	241.1	61.2	60.3
12.07.2005	326.4	57.6	79.9
13.07.2005	305.4	61.6	75.0
14.07.2005	251.7	53.0	62.7
15.07.2005	205.7	71.7	52.1
18.07.2005	347.6	71.2	84.7
19.07.2005	202.7	132.3	51.3
20.07.2005	436.8	66.2	104.6
21.07.2005	293.7	71.1	72.5
22.07.2005	262.0	70.4	65.1
25.07.2005	182.1	98.3	46.7
26.07.2005	310.4	72.9	76.1
27.07.2005	204.2	76.2	51.8
28.07.2005	206.4	68.8	52.7
Average	278.5	70.7	68.9

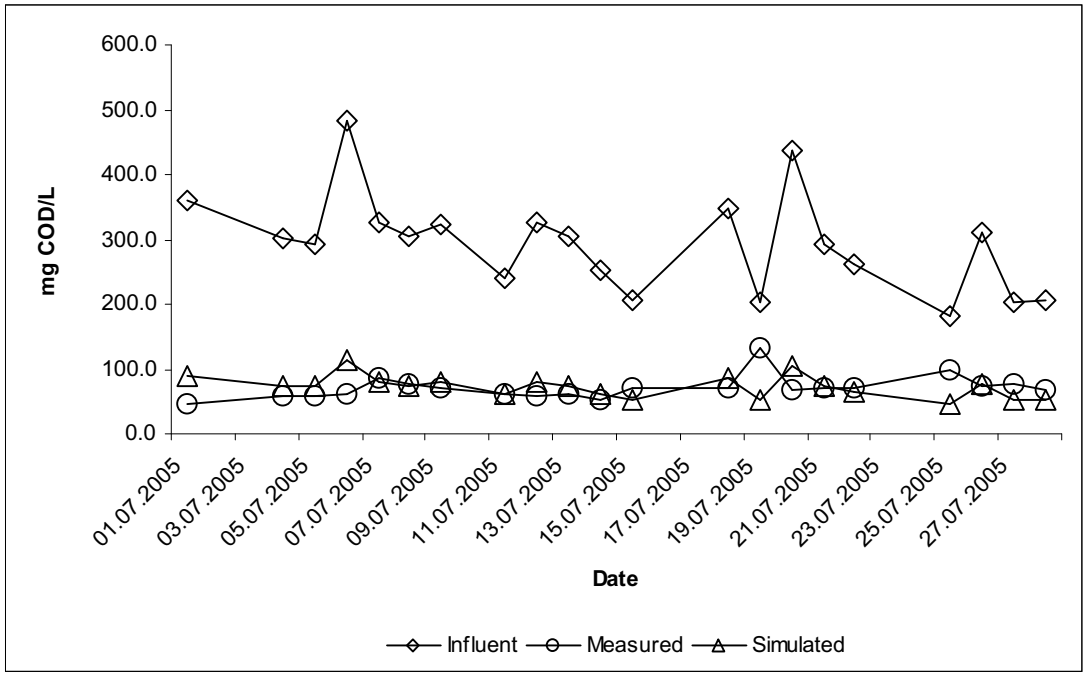


Figure 5.1 Simulation results for COD

Taking into account that an inhibitory effect which probably caused by toxic substances entering the plant between 05.07.05 and 08.07.05, and between 19.07.05 and 21.07.05, it can be easily seen that simulated results reasonably well fitted to the measured actual data. This inhibitory effect is also stated by plant operator. A goodness fit test is applied to measured and simulated results in the following section.

Simulated results for effluent TKN concentrations compared with measured actual plant data are presented in Figure 5.2. These results are also present in a tabular form in Table 5.2.

As mentioned above, an inhibitory effect is present between 05.07.2005 and 08.07.2005. In Figure 5.2, it can be seen that actual effluent TKN concentrations increase significantly between this period while simulation results are linear. While the reason behind the decrement after this period remains unknown, it is probably caused by varying operational strategies. The increment in sludge recycle previously shown in Table 4.1 is thought to be the reason of this decrement.

Table 5.2 Influent, measured and simulated TKN concentrations

	Influent mg/L	Effluent Measured mg/L	Effluent Simulated mg/L
01.07.2005	14.8	2.5	4.8
04.07.2005	16.5	5.9	5.3
05.07.2005	14.3	4.6	5.0
06.07.2005	16.3	8.0	4.6
07.07.2005	15.3	11.9	5.1
08.07.2005	15.8	10.8	5.2
09.07.2005	15.8	9.5	5.2
11.07.2005	14.1	1.4	5.0
12.07.2005	15.0	3.4	5.0
13.07.2005	15.8	4.4	5.2
14.07.2005	15.1	5.9	5.2
15.07.2005	15.3	8.8	5.3
18.07.2005	15.7	11.3	5.1
19.07.2005	16.5	9.6	5.4
20.07.2005	47.3	10.7	6.3
21.07.2005	17.2	13.4	5.4
22.07.2005	16.5	11.3	5.5
25.07.2005	15.2	10.9	5.5
26.07.2005	22.0	6.4	6.0
27.07.2005	14.7	7.9	5.6
28.07.2005	7.7	7.7	3.0
Average	16.9	7.6	5.4

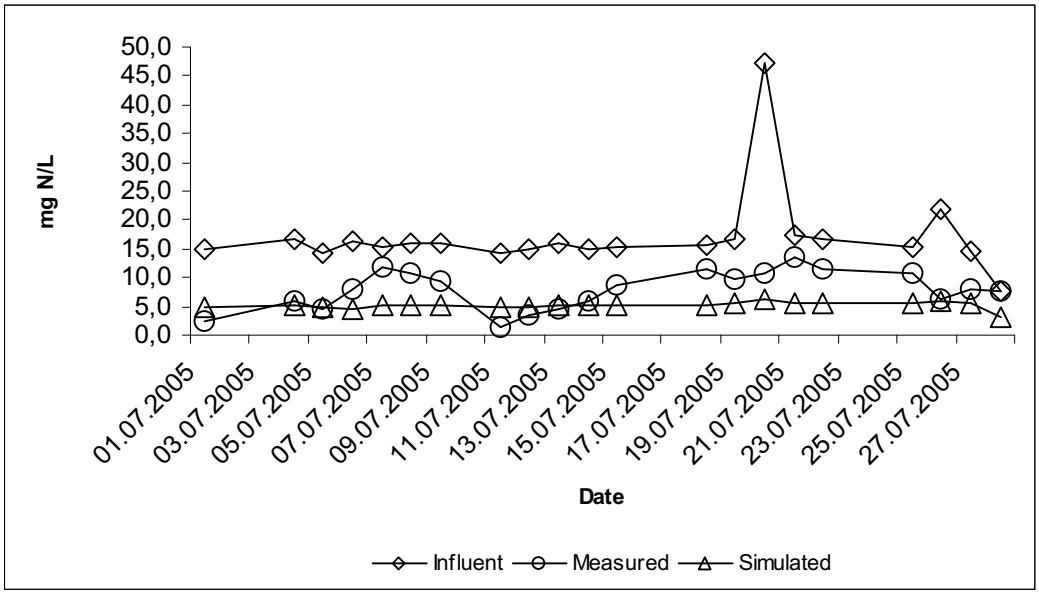


Figure 5.2 Simulation results for TKN

Simulated results for aeration tank MLSS concentration compared with measured actual plant data are presented in Figure 5.3. These results are also presented in a tabular form in Table 5.3.

Table 5.3 Measured and simulated MLSS concentrations in aeration tanks

	Measured mg/L	Simulated mg/L
01.07.2005	4140	3360
04.07.2005	2340	3086
05.07.2005	2060	2556
06.07.2005	1500	4174
07.07.2005	1000	2986
08.07.2005	5100	2818
09.07.2005	4760	2987
11.07.2005	3800	2117
12.07.2005	3620	3057
13.07.2005	3080	2989
14.07.2005	2500	2583
15.07.2005	3100	2099
18.07.2005	3460	3203
19.07.2005	3020	1753
20.07.2005	1620	3873
21.07.2005	3360	2844
22.07.2005	5820	2488
25.07.2005	2940	1681
26.07.2005	3440	2952
27.07.2005	2980	1917
28.07.2005	2860	1972
Average	3127	2586

The inhibition problem previously stated has a more dramatic effect over MLSS. As seen on Figure 5.3, MLSS significantly decreases between indicated periods and requires a longer time to reach normal concentrations and the dramatic increment afterwards indicates that the plant operates highly loaded.

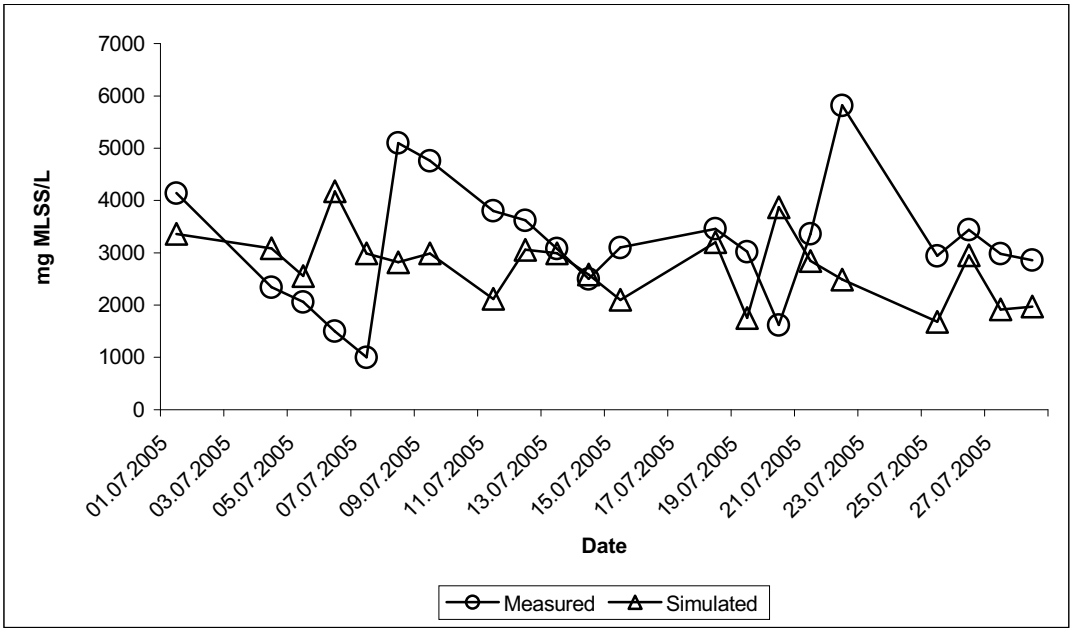


Figure 5.3 Simulation results for MLSS

5.2 Statistical Evaluation of Simulation Results

Chi-squared goodness fit test provides a statistically proved way to test whether data collected in the field does indeed follows a particular theoretical probability distribution (Moore & Cobby, 1988). In this study a chi-squared goodness fit test is employed to test whether the measured data for COD, TKN and MLSS in the plant follow the simulation distribution obtained for these parameters.

5.2.1 Goodness Fit Test for COD

Null and alternative hypothesis are formulated for COD to test whether or not the field data follows the simulation distribution as follows:

H_0 – *COD:* The measured COD in each COD category follows the distribution generated by simulation.

H_1 – *COD:* The measured COD in each COD category does not follow the distribution generated by the simulation.

Data in the inhibitory periods are not included in statistical tests because inhibition can not be defined in the simulation although it has a significant effect on the actual data. Table 5.4 summarizes measured and simulated frequencies for COD data set and finally computing the test χ^2 statistics.

Table 5.4 χ^2 statistics test for COD data set

Median	Measured			Simulated			Total (χ^2)
	O	E	(O-E)2/E	O	E	(O-E)2/E	
<71.2	9	7.5	0.300	6	7.5	0.300	
>71.2	7	8.5	0.265	10	8.5	0.265	
Total			0.565	Total		0.565	1.129

O: Observed E: Expected

As seen on Table 5.4 result of χ^2 statistics yields 1.129 for COD data set. Since degree of freedom (DF) is k-1 where k equals the number of rows, DF is 2-1 = 1. In this case, critical χ^2 value is 10.827 for 0.5 % significance level. In this test, χ^2 statistics is well below the critical value that leads to the conclusion that null hypothesis (H_0) can not be rejected. It is thereby statistically shown that the claim that measured COD data distribution follows the simulated COD data distribution.

5.2.2 Goodness Fit Test for TKN

Null and alternative hypothesis are formulated for TKN to test whether or not the field data follows the simulation distribution as follows:

H_0 – TKN: The measured TKN in each TKN category follows the distribution generated by simulation.

H_1 – TKN: The measured TKN in each TKN category does not follow the distribution generated by the simulation.

Data in the inhibitory periods are not included in statistical tests because inhibition can not be defined in the simulation although it has a significant effect on

the actual data. Table 5.5 summarizes measured and simulated frequencies for COD data set and finally computing the test χ^2 statistics.

Table 5.5 χ^2 statistics test for TKN data set

Median	Measured			Simulated			Total (χ^2)
	O	E	(O-E)2/E	O	E	(O-E)2/E	
<5.4	4	8.5	2.382	6	8.5	2.382	
>5.4	12	7.5	2.700	10	7.5	2.700	
Total			5.082	Total		5.082	10.165

O: Observed E: Expected

As seen on Table 5.5 result of χ^2 statistics yields 10.165 for COD data set. Since degree of freedom (DF) is k-1 where k equals the number of rows, DF is 2-1 = 1. In this case, critical χ^2 value is 10.827 for 0.5 % significance level. In this test, χ^2 statistics is below the critical value that leads to the conclusion that null hypothesis (H_0) can not be rejected. It is thereby statistically shown that the claim that measured TKN data distribution follows the simulated TKN data distribution.

5.2.3 Goodness Fit Test for MLSS

Null and alternative hypothesis are formulated for MLSS to test whether or not the field data follows the simulation distribution as follows:

H_0 – MLSS: The measured MLSS in each MLSS category follows the distribution generated by simulation.

H_1 – MLSS: The measured MLSS in each MLSS category does not follow the distribution generated by the simulation.

Data in the inhibitory periods are not included in statistical tests because inhibition can not be defined in the simulation although it has a significant effect on the actual data. Table 5.6 summarizes measured and simulated frequencies for MLSS data set and finally computing the test χ^2 statistics.

Table 5.6 χ^2 statistics test for MLSS data set

Median	Measured			Simulated			Total (χ^2)
	O	E	(O-E)2/E	O	E	(O-E)2/E	
<2989	5	8	1.125	11	8	1.125	
>2989	11	8	1.125	5	8	1.125	
Total			2.250	Total		2.250	4.500

O: Observed E: Expected

As seen on Table 5.6 result of χ^2 statistics yields 4.500 for MLSS data set. Since degree of freedom (DF) is k-1 where k equals the number of rows, DF is 2-1 = 1. In this case, critical χ^2 value is 10.827 for 0.5 % significance level. In this test, χ^2 statistics is below the critical value that leads to the conclusion that null hypothesis (H_0) can not be rejected. It is thereby statistically shown that the claim that measured MLSS data distribution follows the simulated MLSS data distribution.

5.3 Determination of Organic Capacity of The Plant

A series of simulation studies is performed in order to determine the amount for carbonaceous material that Güneybatı WWTP can handle. An average flowrate of 16369 m^3/day is used in simulation studies.

Plant's organic capacity is determined considering two limits: the effluent COD concentration and the amount of oxygen that can be transferred into the wastewater. Legal limit of 140 mg COD/L stated in table 21.3 of Water Pollution Control Directive is accepted as the effluent limit for the plant. Total oxygen transfer capacity is determined according to the blower capacity of the plant.

As previously mentioned under title 4.1, plant operates 5 blowers each with a capacity of 2250 m^3/h which totals 11250 m^3/h. Assuming that the air includes 21% of oxygen, molecular weight of oxygen is 32 g/mole, 1 mole of gas fills 22.4 L in standard conditions and oxygen transfer efficiency is 0,08 (Tchobanoglous & Burton, 2003), the following calculation is performed.

$$OC = 0.08 \frac{11250 m^3/h x 0.021 x 1000 L/m^3 x 32 g/mole}{22.4 L/mole x 1000 g/kg} x 24 h/d = 6480 kg/d \quad (4.1)$$

Simulation studies are started with 300 mg COD/L –just above the monthly average- and resulted with 1000 mg/L. Monthly average nitrogenous component concentrations given in Table 4.5 are used in the simulations.

Results of the simulation studies are summarized in Table 5.7. Filled cells shows the conditions that plant capacity is exceeded either by oxygen consumption or effluent COD.

Table 5.7 Results of simulation studies

Influent COD (mg/L)	300	400	500	600	700	800	900	1000
Effluent COD (mg/L)	73.9	96.9	119.9	142.9	165.9	188.9	211.9	234.9
MLSS (mg/L)	2340.3	3143.9	3945.0	4750.4	5563.8	6371.8	7169.2	7965.7
O2 Consumption (kg/d)	2295.4	2906.2	3528.5	4161.4	4807.7	5483.7	6176.7	6870.9

As it can be seen from the table plant can handle up to 900 mg/l of COD to meet the discharge limit of 140 mg/L while the oxygen transfer capacity of the plant is enough to treat wastewater with 900 mg/L of COD. Results of simulation studies are presented in Figures 5.4 and 5.5

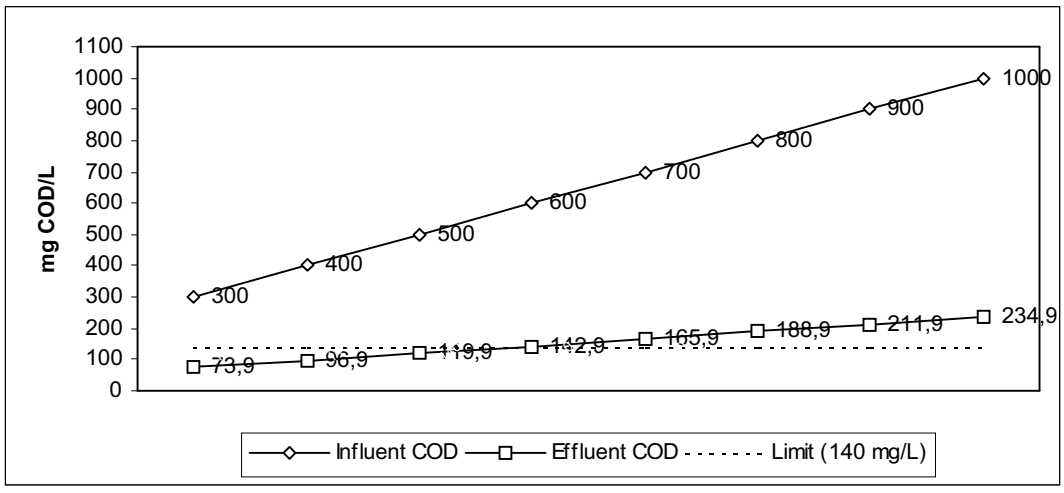


Figure 5.4 Simulation results with COD as the limiting factor.

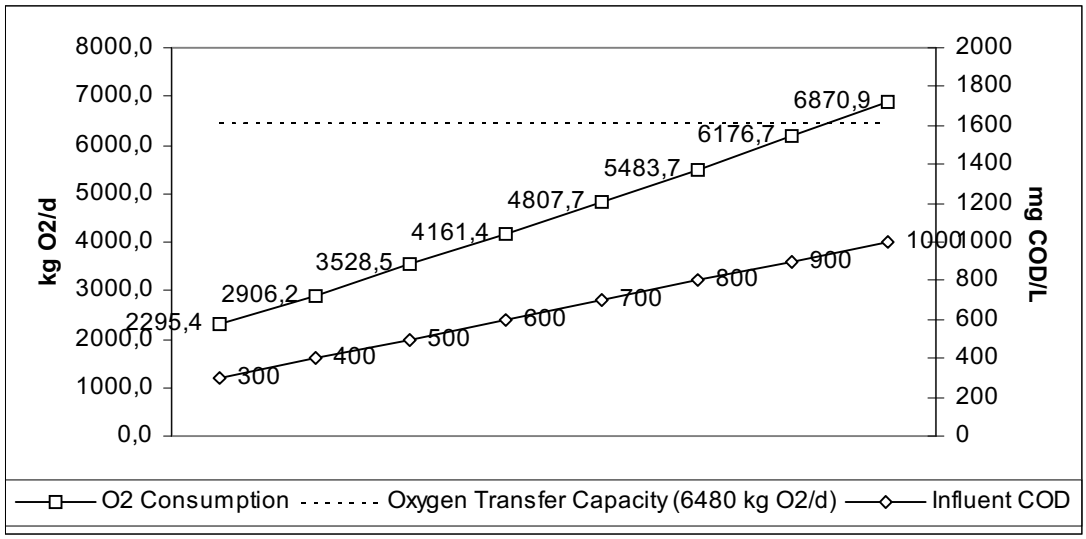


Figure 5.5 Simulation results with oxygen consumption as the limiting factor.

These results have shown that the plant can be safely operated with the average flowrate to treat up to 600 mg/L of COD and the five blowers of 2250 m3/h are enough to supply necessary oxygen to treat 900 mg/L of COD.

CHAPTER SIX
CONCLUSIONS

In this study, IWAQ Activated Sludge Model Number 1 (ASM1) was applied to İzmir Güneybatı Wastewater Treatment Plant using Single-sludge Simulation Program (SSSP) as the simulation environment. Different determination methods for wastewater fractions and kinetic and stoichiometric parameters are evaluated and wastewater is fractionated.

As a result of study, it is shown that the fate of carbonaceous and nitrogenous components of wastewater together with MLSS concentration in aeration tanks can be simulated using ASM1 except for the inhibitory conditions. Results of simulation and data obtained from plant effluent significantly differ from each other when toxic compounds are present in the influent and for some parameters, like MLSS, several days may be required to recover normal operation conditions.

Although kinetic and stoichiometric parameters are not experimentally determined, model predictions reasonably fitted to actual data. Therefore it may be concluded that ASM1 model successfully describes biochemical reactions taking place in activated sludge processes.

Further calibration studies such as experimental determination of wastewater fractions and sensitive kinetic and stoichiometric model parameters and dynamic calibration must be conducted in order to define processes more preciously. After calibration, model can be used in evaluating different operational and control strategies towards improving plant efficiency.

ASM1, when calibrated and verified, can be used for maintaining optimum operational conditions as well as estimating plant's response to varying wastewater characteristics. Hydraulic and organic capacities of the plant can also be estimated to aid operators to take precautions before loss of biomass occurs.

With the aid of simulation studies, it's determined that the plant can be safely operated to treat 600 mg/L of COD which doubles the monthly average, and the blower capacity of the plant is sufficient to treat this COD.

It is recommended that mathematical models such as ASM1, which was evaluated in this study, should be used widely in both and design of activated sludge plants for improving treatment efficiency and reducing operational costs. Combined with a secondary clarifier model, ASM1 will successfully meet the demands of operators for efficient and optimum plant operation.

Finally, it should be noted that ASM1 model is by no means complete and operators of the model are required to have necessary background knowledge and more precious calibration studies should be employed before actual application of model to the plant conditions at full-scale.

REFERENCES

de la Sota A., Larrea L., Novak L., Grau P. & Henze M., 1994 Performance and model calibration of R-D-N processes in pilot plant. *Water Sci. Technol.*, 30(6), 355 – 364.

Dold, P.L., Ekama, G.A.,& Marais, G.v.R., 1980, A general model for the activated sludge process., *Prog. Wat. Tech.*, 12, 47-77.

Drolka, M., Plazl, I., & Koloini, T., 2001, The results of mathematical model and pilot plant research of wastewater treatment. *Model and Wastewater Treatment*., 15(2), 71 – 74.

Dupont R., & Sinkjær O., 1994, Optimization of wastewater treatment plants by means of computer models. *Water Sci. Technol.*, 30(4), 181 – 190.

Grady, C.P.L.Jr., Daigger, G.T., & Lim, H.C., 1999, *Biological wastewater treatment*, NY: Marcel Dekker Inc.

Henze M., Grady, C.P.L., Gujer, W., Marais, G.v.R., & Matsuo, T., 1987, Activated sludge model no 1 by IAWQ task group on mathematical modeling for design and operation of biological wastewater treatment. *Scientific and Technical Reports No 1.* London: IAWQ

Henze, M., 1992, Characterization of wastewater for modeling activated sludge processes. *Water Sci. Technol.* 25(6), 1 – 15.

Henze M., Gujer W., Mino T., Matsuo T., Wentzel M.C.M. & Marais G.v.R., 1995, Activated sludge model no 2. *IAWQ Scientific and Technical Report No. 3*, London: IAWQ

Henze M., Gujer W., Mino T., Matsuo T., Wentzel M.C., Marais G.v.R. & van Loosdrecht M.C.M., 1999, Activated sludge model No. 2D, ASM2D. *Water Sci. Technol*., 39(1), 165 – 182.

Jeppsson, U. *Modeling aspects of wastewater treatment processes*., PhD Thesis, Dept. Of Industrial Electrical Engineering and Automation, Lund: Lund University.

Kappeler, J., & W. Gujer, 1992, Estimation of kinetic parameters of heterotrophic biomass under aerobic conditions and characterization of wastewater for activated sludge modeling, *Wat. Sci.Techn.* 25, 125-139.

Kristensen H.G., la Cour Janssen J. & Elberg Jørgensen P., 1998, Batch test procedures as tools for calibration of the activated sludge model – A pilot scale demonstration. *Water Sci. Technol.*, 37(4-5), 235 – 242.

Lesouef A., Payraudeau M., Rogalla F. & Kleiber B., 1992, Optimizing nitrogen removal reactor configurations by on-site calibration of the IAWPRC activated sludge model. *Water Sci. Technol*., 25(6), 105 – 123.

Mamais D., Jenkins D. & Pitt P., 1993, A rapid physical-chemical method for the determination of readily biodegradable soluble COD in municipal wastewater., *Water Res.*, 27, 195 – 197.

Marsili-Libelli, S., & Tabani, F., 2001, Accuracy analysis of a respirometer for activated sludge dynamic modeling. *Water Research*, 36, 1181-1192.

Nowak O., Franz A., Svardal K., Muller V., & Kuhn., 1999, Parameter estimation for activated sludge models with help of mass balances. *Water Sci. Technol*., 39(4), 113 – 120.

Orhon, D., & Artan, N., 1994, *Modeling of activated sludge systems*., London : Technomic Publishing Inc.

Petersen, B., 2000, *Calibration, identifiability and optimal experimental design of activated sludge process*. PhD Thesis, Dept. Of Industrial Electrical Engineering and Automation, Lund: Lund University.

Sin, G., 2000, *Determination of ASM1 sensitive parameters and simulation studies for Ankara wastewater treatment plant*. M.Sc. Thesis, Graduate School of Natural and Applied Sciences, Ankara: METU

Sin, G., 2004 *Systematic calibration of activated sludge systems*., Ph.D Thesis, Dept. Of Industrial Electrical Engineering and Automation, Lund: Lund University.

Sollfrank, U., & Gujer, W., 1991, Characterization of domestic wastewater for mathematical modeling of the activated sludge process. *Wat. Sci. Tech.* 23 (4-6): 1057-1066.

Tchobanoglous, G., & Burton F.L., 2003, *Wastewater engineering: Treatment, disposal and reuse* (4th ed.) Metcalf and Eddy Inc., NY: McGraw-Hill.

Xu S., & Hultman B., 1996, Experiences in wastewater characterization and model calibration for the activated sludge process. *Water Sci. Technol.* 33(12), 89 – 98.