Combining an Activated Sludge Model with Computational Fluid Dynamics

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Summary

In a modern wastewater treatment plant activated sludge is used for cleaning wastewater. In 1987 the International Association on Water Quality (IAWQ) introduced a mathematical model, Activated Sludge Model No. 1 (ASM1), describing the biological processes in a tank of the treatment plant. In such a tank fluid flow plays an important role. Using Computational Fluid Dynamics this flow can be computed. Both models work separately very well in practice, but what happens if we combine these two models?

It turns out that both models can be coupled using the Navier-Stokes equations for fluid flow and convection-diffusion equations for Activated Sludge Model No. 1. This combined model can be made using COMSOL Multiphysics. A simple two-dimensional model for a tank of a treatment plant will be discussed. This model is also extended with an aeration process, which gives the flow a turbulent character.
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Chapter 1

Introduction

Have you ever wondered what happens with the water when you flush the toilet? And did you know that mathematics can play a role?

The answer to these simple questions are one of the main subjects of this thesis. When flushing a toilet or when water is thrown away through the sink, the water with its pollution enters the sewer. From here it is transported to a wastewater treatment plant (WWTP). This installation is developed for the treatment of wastewater. It cleans the water before it is discharged in nature. In modern plants biological processes are used for the removal of organic material, nitrogen and phosphorus. Such a treatment plant uses activated sludge.

In the last 25 years the (mathematical) modelling of a wastewater treatment plant has become an important subject in the optimization and design of a treatment plant. In 1983 the International Association on Water Pollution Research and Control, IAWPRC (later this changed in International Association on Water Quality, IAWQ) formed a task group for the development of mathematical model for wastewater treatment plants. This task group started with the review of existing models and introduced Activated Sludge Model No. 1 (ASM1) in 1986. The model describes biological processes like carbon oxidation, nitrification and denitrification for a treatment plant, which uses activated sludge. In 1995 the task group introduced Activated Sludge Model No. 2 (ASM2), adding biological phosphorus removal to the model. The latest Activated Sludge Models, ASM2d and ASM3, are both introduced in 1999.

In mathematics, Computational Fluid Dynamics (CFD) has become very important for the computations of fluid flows. The basis of CFD are the Navier-Stokes equations, derived by Claude-Louis Navier and George Stokes in the nineteenth century. Because it is hard to solve them with pen and paper, numerical methods are developed to solve the equations. Many computer packages are available, for example COMSOL Multiphysics 3.5a.
1.1 Description of the problem

The Activated Sludge Models describe the biological processes in a wastewater treatment plant. The modelling of fluid flow in the tanks of a treatment plant is done using the ‘tanks-in-series’ model, where a few simplifying assumptions in ASM are made. With the development of Computational Fluid Dynamics, it is also possible to compute the fluid flow in tanks of a wastewater treatment plant, giving more realistic results.

Both models work separately very well for treatments plants. But what if we combine an Activated Sludge Model with Computational Fluid Dynamics? Of course, this question is very general. Therefore some more precise questions can be formulated. The most important are:

1. Is it in theory possible to use the equations of one of the Activated Sludge Models in combination with Computational Fluid Dynamics? Is it necessary to modify these equations? Is it possible to numerically solve the equations?

2. The ASM models are developed for the use with the tanks-in-series model. The tanks-in-series model can be seen as a discrete model for the flow in tanks. A CFD-model is a continuous model for the complete tank. Does this give any problems in the implementation of the models?

3. All ASM models are relative large models as we will see in the next chapter, with many components (varying from 10 to 21) and processes (varying from 8 to 21). Are all these processes necessary to implement together with a CFD model? Is it possible to simplify the ASM models in such a way that the model becomes smaller, but still gives the desired results? Are all ASM models applicable with CFD?

4. What kind of model is needed to describe the flow in a reactor? Can the incompressible Navier-Stokes equations be used? Do we need a turbulence model?

5. The activated sludge tank of a wastewater treatment plant contains aerated parts, to create aerobic, anoxic and anaerobic environments. How can we model this aeration in a CFD model?

6. Do the results of the combined model represent the real world?

7. What are the benefits and drawbacks of this combination?

In this thesis we will try to give an answer to these questions. The problem described above was introduced by Witteveen+Bos, an engineering company located in Deventer (The Netherlands).
1.2 Outline of the thesis

In the next chapters we try to find an answer to the questions formulated in the previous section. First the Activated Sludge Models are introduced. All components and processes in the model will be shortly discussed. In the chapter that follows the modelling of fluid flow is the main subject. The tanks-in-series model will be discussed, followed by a description of the Navier-Stokes equations. Also a turbulence model is introduced. The chapter ends by introducing a model for mass transport and mass transfer.

The models made for this thesis are implemented with COMSOL Multiphysics. This computer program uses the finite element method for solving partial differential equations. In chapter 4 a short description of this method is given. In the next chapter Activated Sludge Model No. 1 is combined with CFD. First the theory of this combination is discussed, followed by some simple models of a wastewater treatment plant. The results of these models are treated in chapter 6.

The conclusions and a discussion of complete project can be found in the final chapter. Also recommendations for future work are given. In the appendix, at the end of the thesis a step-by-step description can be found for making a model in COMSOL.
CHAPTER 1. INTRODUCTION
Chapter 2

A Description of the Activated Sludge Models

In this chapter the Activated Sludge Models will be introduced. The mathematical models are developed by the International Association on Water Quality (IAWQ). Before looking at the models, first the biological processes in a wastewater treatment plant are introduced. This is followed by a small introduction about the notation of the models. Also the basic principles behind the Activated Sludge Models will be discussed here.

For every sludge model, ASM1, ASM2, ASM2d and ASM3 all relevant information will be given. Also some limitations of the models will discussed. Finally a short comparison is made between the four models.

2.1 Processes in a Wastewater Treatment Plant

Before looking at the processes in a wastewater treatment plant, it is important to know what components can be found in the water. The pollution is mainly formed by organic compounds, nitrogen and phosphorus. Nitrogen appears in terms of nitrate and ammonia. And the organic compounds exist out hydrocarbons.

When wastewater from the sewer enters a treatment plant, the water is filtered. Large particles in the wastewater are removed immediately. Then the water enters the tanks of the wastewater treatment plant where biological and chemical processes play an important role. Biological processes remove the pollution from the wastewater. In most treatment plants this is done using activated sludge. In this sludge there are micro-organisms, like bacteria, which assist with the clean up in the wastewater [15].

The biological reactions performed by the organisms in the activated sludge can be divided into two types [5]. First, there are aerobic reactions, where the bacteria need oxygen to perform the reactions. These bacteria are also called heterotrophs. The other type of reaction is the anaerobic reaction, where oxygen ($O_2$) is not needed. Bacteria
performing anaerobic reactions are also called autotrophs. Both type of bacteria play an important role in the treatment of wastewater.

Organic compounds in wastewater are treated with aerobic bacteria. These bacteria use the organic components in the wastewater for their growth and energy supply. The organic material is transformed into (gas) carbondioxide and water. For this process oxygen is needed. Because the water contains different organic components, one example is given. Consider the treatment of ethanol, with the reaction equations
\[
\begin{align*}
\text{CH}_3\text{CH}_2\text{OH} + O_2 & \rightarrow \text{CH}_3\text{COOH} + H_2O, \\
\text{CH}_3\text{COOH} + 2O_2 & \rightarrow 2\text{CO}_2 + 2H_2O.
\end{align*}
\]

The heterotrophic bacteria transform the organic compound in the wastewater in a two-step process in water and carbondioxide.

The second process in a WWTP is nitrification. In this two-step process the ammonium in wastewater is removed by a transformation into nitrate. This is a two-step process, because ammonium is transformed into nitrite and this is again transformed into nitrate. For the removal process the chemical equations are
\[
\begin{align*}
2\text{NH}_4^+ + 3O_2 & \rightarrow 2\text{NO}_2^- + 2H_2O + 4H^+, \\
2\text{NO}_2^- + O_2 & \rightarrow 2\text{NO}_3^-.
\end{align*}
\]

As can be seen in the chemical equations both processes require oxygen. The first process is done by the *Nitrosomonas* bacteria and the second process by the *Nitrobacter* bacteria.

Another process in a wastewater treatment plant is denitrification. This process is related to the nitrification process. One major difference with the previous processes is the fact that denitrification is an anaerobic process and thus performed by autotrophic bacteria. These bacteria do not need oxygen to perform the transformation from nitrate into nitrogen. The chemical equation of denitrification is given as
\[
2\text{NO}_3^- + 2H^+ \rightarrow N_2 + 5O + H_2O.
\]

Together with this denitrification there is a process transforming some organic compound into carbondioxide and water, using the oxygen produced in the denitrification. For completeness, this chemical equation is given as
\[
\text{organic compound} + 5O \rightarrow \text{CO}_2 + H_2O.
\]

One remark for this equations is that oxygen is always bounded as $O_2$. The term $5O$ in above equations can also be replaced by $2.5O_2$. These reaction equations only give a general idea. The amount of oxygen needed to transform organic compound is probably larger than $5O$. Also amount of carbondioxide and water will be larger.

The removal of phosphorus (and/or phosphate) has become an important process in the wastewater treatment. There are two ways to remove the phosphorus. One biological
way and a chemical way. This chemical process requires the use of a metal ion, in most cases calcium ($Ca^{2+}$), aluminium ($Al^{3+}$) or iron ($Fe^{3+}$). In the activated sludge models it is assumed to use iron. The corresponding chemical equation is given as

$$Fe^{3+} + H_nPO_4^{3-n} \leftrightarrow FePO_4 + nH^+,$$

where $n = 0, 1, 2, 3$.

The processes described above are only a selection of the biological processes in the wastewater treatment. There are also some other processes. An example of such a process is the hydrolysis of some (organic) material. Hydrolysis is a process that, with the help of enzymes, large organic compounds transforms into smaller organic compounds. It can be seen as a process that splits chemical bounds in large organic molecules. The relatively large compounds are not suitable for the processes in wastewater treatment described above. The smaller organic compounds however, can be used in the processes of wastewater treatment. Other processes in a treatment plant are the removal of sulphate and the oxidation of sulphur. Both will not be treated in the Activated Sludge Models.

2.2 Basis of the Model and Notation

A mathematical model must be representative for most important fundamental processes within a system. A process is an event on one or more components of a system, in this case a wastewater treatment plant (WWTP). The Activated Sludge Models describe the biological processes in a treatment plant. The physical basis for the models are mass-balance equations. These equations hold in a certain domain, for example a tank of a WWTP, and have the general form

$$\text{Input} - \text{Output} + \text{Reaction} = \text{Accumulation}. \quad (2.1)$$

In this equation the input and output are the so-called transport terms, which depend on the physical characteristics of a system. The reaction term represents all chemical and biological processes within the system. In a steady state situation the accumulation term is assumed to be zero.

All four activated sludge models, introduced by the IAWQ task group, use a matrix format notation. To understand the matrix notation a small example will be treated. Consider therefore heterotrophic bacteria growing in an aerobic environment using soluble carbon substrate and oxygen. Substrate is a general name for (organic) material, which can be transformed by a biological process. This process could be performed with help of enzymes.

The two fundamental processes for this example are the growth and decay of bacteria (increase and decrease of biomass). Also the events of oxygen utilization and substrate removal should treated, because both are used for the growth of bacteria. This immediately means that the concentrations of substrate and oxygen should decrease. The model
introduced here must contain at least the components biomass (bacteria), substrate and dissolved oxygen. In Table 2.1 the matrix notation can be found for the model of aerobic growth of heterotrophic bacteria. Below the matrix a detailed description will be given.

<table>
<thead>
<tr>
<th>Component (i) →</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>process rate $\rho_j$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process (j) ↓</td>
<td>$X_B$</td>
<td>$S_S$</td>
<td>$S_O$</td>
<td>$[ML^{-3}T^{-1}]$</td>
</tr>
<tr>
<td>1. Growth</td>
<td>1</td>
<td>$-\frac{1}{Y}$</td>
<td>$-\frac{1-Y}{Y}$</td>
<td>$\left(\frac{\mu S_S}{K_S+S_S}\right) X_B$</td>
</tr>
<tr>
<td>2. Decay</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>$b X_B$</td>
</tr>
</tbody>
</table>

Observed Conversion Rates $[ML^{-3}T^{-1}]$  
$r_i = \sum_j \nu_{ij} \rho_j$

Stoichiometric parameters:
- True growth yield, $Y$
- Biomass $\frac{M(COD)}{L^3}$
- Substrate $\frac{M(COD)}{L^3}$
- Oxygen $\frac{M(-COD)}{L^3}$ (negative COD)

Kinetic parameters:
- Max. specific growth rate, $\mu$
- Half-velocity constant, $K_S$
- Specific decay rate, $b$

Table 2.1: Matrix notation for growth of heterotrophic bacteria in an aerobic environment. The definition of parameters $Y, \mu, K_S, b$ is given in the table. $M(COD)$ is a unit of weight, the weight of the material is expressed in terms of the weight of Chemical Oxygen Demand (COD). COD is explained in the text. $L$ is the unit of length. It is not chosen here, it could be in metres, or in centimetres. $L^3$ represents a volume. $T$ is the unit of time, again this is not yet determined. In most cases time is expressed in hours.

In the first row of Table 2.1 the components of the model can be found. Here $X$ stands for insoluble (particulate) elements and $S$ stands for soluble elements. Using the subscript notation all individual components are specified, in this case $B$ is biomass, $S$ is substrate and $O$ is oxygen. All components are given the index $i$ in this model representation. Next the biological processes, with index $j$, are presented in the first column of the table. In this example these processes are the growth of biomass and the loss of biomass due to decay.

The notation with indices $i,j$ are an essential part of the matrix notation. In a matrix the indices determine the exact element in that matrix. For example, in a 5 by 5 matrix with real numbers, if $i,j = 2,3$ then the element in the second row and third column of the matrix is meant. This is also valid for the matrix notation in Table 2.1 but here the matrix is filled with parameters and represents a biological model.

The kinetic expressions, or rate equations, for each process in the model are listed in the last (rightmost) column of the table. These process rates are denoted by $\rho_j$, with $j$ the number of the corresponding process. The rates in Table 2.1 are defined using a simple Monod model. Monod’s growth model is an empirical model describing the micro-biological growth (see for example). The model relates the growth rate and the concentration of...
2.2. BASIS OF THE MODEL AND NOTATION

A limiting nutrient (element in the substrate). The model is given by the equation

\[ \frac{dx}{dt} = x \mu_m \frac{s}{K_s + s}, \] (2.2)

where \( x \) is the biomass and \( s \) the limiting substrate. \( \mu_m \) is the maximum specific growth rate and \( K_s \) the concentration of substrate, which supports the half-maximum growth rate (or the half saturation rate constant of substrate). In table 2.1 it is evident that the Monod model is used in the rate equations.

In this model \( \rho_1 \) is the process rate for the growth of biomass, which is proportional to the biomass concentration \( (X_B) \) in a first order manner and to the substrate concentration \( (S_S) \) in a mixed order manner, using the Monod model. Process rate \( \rho_2 \) says that the biomass decay is of the first order with respect to biomass concentration.

The elements in the matrix are the stoichiometric coefficients \( \nu_{ij} \). They give the mass relationships between the components in the individual processes in the model. The coefficients are greatly simplified. If a coefficient is positive, it means that there is a production of material. If, however, the coefficient in the matrix is negative, then we speak of consumption. In table 2.1 we see that the growth of biomass \( (\nu_{11} = +1) \) occurs with the consumption of substrate \( (\nu_{12} = -\frac{1}{Y}) \) and oxygen \( (\nu_{13} = -\frac{1}{Y}) \).

With the matrix in table 2.1 the mass-balance equations can be made. The matrix gives the reaction terms for the model. These terms can be found using the following formula,

\[ r_i = \sum_j \nu_{ij} \rho_j, \text{ for each component } i. \] (2.3)

For example, the reaction term in the mass-balance of the biomass \( (X_B) \) is \( r_{X_B} = \frac{\mu S_S X_B}{K_S + S_S} - bX_B \). So, for each component in the model, the reaction term in the mass-balance equation can be found by summing over the column of the matrix. The stoichiometric parameter is multiplied with the corresponding rate equation. Then the summation over all terms is performed.

Now, we look to the simple model given in the matrix. Consider the heterotrophic bacteria (biomass). Assume that in a tank, there is no inflow or outflow, so in equation 2.1 input and output are zero. What remains are the accumulation and reaction terms. The total equation for the biomass concentration becomes

\[ \frac{dX_B}{dt} = \left[ \mu \frac{S_S}{K_S + S_S} - b \right] X_B. \] (2.4)

In a similar way we get equations for the substrate and oxygen concentrations, given as (still without in- and outflow)

\[ \frac{dS_S}{dt} = -\frac{\mu}{Y} \frac{S_S}{K_S + S_S} X_B, \] (2.5)

\[ \frac{dS_O}{dt} = \left[ -\mu \frac{1 - Y}{Y} \frac{S_S}{K_S + S_S} - b \right] X_B. \] (2.6)
CHAPTER 2. A DESCRIPTION OF THE ACTIVATED SLUDGE MODELS

So, the simple model given in table 2.1 contains three equations describing the growth and decay of heterotrophic biomass.

One final remark about the matrix notation is the fact that continuity of the model can easily be checked. If consisted units are used for the elements in the matrix, then the sum over all stoichiometry coefficients ($\nu_{ij}$) from one process must be zero. So summing the elements in one row of the matrix should give zero. We have to keep in mind that the sign of the parameter can change with production or consumption.

2.3 Activated Sludge Model No. 1

The first model introduced for modelling the processes in a wastewater treatment plant is the Activated Sludge Model No. 1. Before looking at the matrix of ASM1, first the concept of a switching function is introduced. Switching functions are the basis of the Monod model. These functions are used in the process rate equations and are able to turn them on and off, if environmental conditions are changed. Consider, for example, the bacteria for nitrification. They grow under aerobic conditions, but if the amount of dissolved oxygen approaches zero, the biomass stops growing. The switching function introduced is

$$S_O \quad (2.7)$$

where $S_O$ is the concentration of dissolved oxygen and $K_O$ the half maximum growth rate constant. If $K_O$ almost equals zero, the switching function is almost 1 and if the amount of dissolved oxygen approaches zero, the function also becomes zero. If there is no oxygen at all the switching function

$$K_O \quad (2.8)$$

can be used. Both functions are continuous, which helps to eliminate problems with numerically instability. The complete Activated Sludge Model No. 1 can be found in the tables 2.2 and 2.3 where the matrix notation is used. In this section AMS1 is further described.

2.3.1 Components in ASM1

In ASM1 all mass-balances can be made using Chemical Oxygen Demand (COD). All organic materials can be expressed in terms of COD units. Chemical Oxygen Demand is an indirect measure of the organic compounds in the wastewater. It measures the requirement of oxygen used for oxidation, hydrolysis and fermentation of organic material in the water. In ASM1 the organic matter may be subdivided into a number of categories. First there is the non-biodegradable material, which is subdivided into soluble ($S_I$) and particulate ($X_I$) inert organic matter. Then there is the biodegradable material, or substrate. This is again subdivided in readily biodegradable substrate ($S_S$) and slowly biodegradable substrate
2.3. ACTIVATED SLUDGE MODEL NO. 1

<table>
<thead>
<tr>
<th>Comp. ( i \rightarrow j ) Process ↓</th>
<th>( S_I )</th>
<th>( S_J )</th>
<th>( X_I )</th>
<th>( X_J )</th>
<th>( X_{B,H} )</th>
<th>( X_{B,A} )</th>
<th>( X_P )</th>
<th>( S_O )</th>
<th>( S_{NO} )</th>
<th>( S_{NH} )</th>
<th>( S_{ND} )</th>
<th>( X_{ND} )</th>
<th>( S_{ALK} )</th>
<th>( \rho_i )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Aerobic growth heterotrophs</td>
<td>( \frac{-1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>1</td>
<td>( \frac{1}{Y_H} )</td>
<td>( 1 )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
</tr>
<tr>
<td>2. Anoxic growth heterotrophs</td>
<td>( \frac{-1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>1</td>
<td>( \frac{1}{Y_H} )</td>
<td>( 1 )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
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<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
</tr>
<tr>
<td>3. Aerobic growth autotrophs</td>
<td>( \frac{1}{Y_A} )</td>
<td>( \frac{1}{Y_A} )</td>
<td>( \frac{1}{Y_A} )</td>
<td>( \frac{1}{Y_A} )</td>
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<td>( \frac{1}{Y_A} )</td>
<td>( \frac{1}{Y_A} )</td>
</tr>
<tr>
<td>4. Decay of heterotrophs</td>
<td>( \frac{1}{f_P} )</td>
<td>( \frac{1}{f_P} )</td>
<td>( \frac{1}{f_P} )</td>
<td>( \frac{1}{f_P} )</td>
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<tr>
<td>5. Decay of autotrophs</td>
<td>( \frac{1}{f_P} )</td>
<td>( \frac{1}{f_P} )</td>
<td>( \frac{1}{f_P} )</td>
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</tr>
<tr>
<td>6. Ammonification of soluble organic nitrogen</td>
<td>( \frac{1}{K_{NO,H}+S_{NO}} )</td>
<td>( \frac{1}{K_{NO,H}+S_{NO}} )</td>
<td>( \frac{1}{K_{NO,H}+S_{NO}} )</td>
<td>( \frac{1}{K_{NO,H}+S_{NO}} )</td>
<td>( \frac{1}{K_{NO,H}+S_{NO}} )</td>
<td>( \frac{1}{K_{NO,H}+S_{NO}} )</td>
<td>( \frac{1}{K_{NO,H}+S_{NO}} )</td>
<td>( \frac{1}{K_{NO,H}+S_{NO}} )</td>
<td>( \frac{1}{K_{NO,H}+S_{NO}} )</td>
<td>( \frac{1}{K_{NO,H}+S_{NO}} )</td>
<td>( \frac{1}{K_{NO,H}+S_{NO}} )</td>
<td>( \frac{1}{K_{NO,H}+S_{NO}} )</td>
<td>( \frac{1}{K_{NO,H}+S_{NO}} )</td>
<td>( \frac{1}{K_{NO,H}+S_{NO}} )</td>
</tr>
<tr>
<td>7. Hydrolysis of entrapped organics</td>
<td>( 1 )</td>
<td>( 1 )</td>
<td>( 1 )</td>
<td>( 1 )</td>
<td>( 1 )</td>
<td>( 1 )</td>
<td>( 1 )</td>
<td>( 1 )</td>
<td>( 1 )</td>
<td>( 1 )</td>
<td>( 1 )</td>
<td>( 1 )</td>
<td>( 1 )</td>
<td>( 1 )</td>
</tr>
<tr>
<td>8. Hydrolysis of entrapped organic nitrogen</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

Table 2.2: All parameters, with components and processes of Activated Sludge Model No. 1. The corresponding process rates can be found in table 2.3.

<table>
<thead>
<tr>
<th>Process rate ([ML^{-3}T^{-1}])</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \rho_1 )</td>
<td>( \mu_H \left( \frac{S_S}{K_S+S_S} \right) \cdot \left( \frac{S_O}{K_{O,H}+S_O} \right) X_{B,H} )</td>
</tr>
<tr>
<td>( \rho_2 )</td>
<td>( \mu_H \left( \frac{S_S}{K_S+S_S} \right) \cdot \left( \frac{S_{NO}}{K_{NO,H}+S_{NO}} \right) \cdot \left( \frac{S_{NO}}{K_{NO,A}+S_{NO}} \right) \eta_B X_{B,H} )</td>
</tr>
<tr>
<td>( \rho_3 )</td>
<td>( \mu_A \left( \frac{S_{NO}}{K_{NO,H}+S_{NO}} \right) \cdot \left( \frac{S_{NO}}{K_{NO,A}+S_{NO}} \right) X_{B,A} )</td>
</tr>
<tr>
<td>( \rho_4 )</td>
<td>( \beta_H X_{B,H} )</td>
</tr>
<tr>
<td>( \rho_5 )</td>
<td>( \eta_A X_{B,A} )</td>
</tr>
<tr>
<td>( \rho_6 )</td>
<td>( \beta_{NO,H} X_{B,H} )</td>
</tr>
<tr>
<td>( \rho_7 )</td>
<td>( \beta_{NO,A} X_{B,A} )</td>
</tr>
<tr>
<td>( \rho_8 )</td>
<td>( \beta_{NO,A} X_{B,A} )</td>
</tr>
</tbody>
</table>

Table 2.3: All process rates for Activated Sludge Model No. 1.
(\(X_S\)), which is treated as particulate material. The hydrolysis process transforms slowly biodegradable substrate into readily biodegradable substrate.

ASM1 also contains nitrogenous matter. Again this is divided in biodegradable and non-biodegradable components. The non-biodegradable material is subdivided into soluble and particulate material. However, since the fraction of non-biodegradable soluble nitrogen is small this is not included in the model. Also, the non-biodegradable particulate nitrogen is associated with the non-biodegradable particulate COD. The biodegradable material consists of ammonia NH (\(S_{NH}\)), nitrate nitrogen NO (\(S_{NO}\)), soluble organic nitrogen (\(S_{ND}\)) and particulate organic nitrogen (\(X_{ND}\)).

Of course, ASM1 also contains biomass. In the model, biomass is divided in two groups, the heterotrophic and autotrophic biomass, \(X_{B,H}\) and \(X_{B,A}\) respectively. The heterotrophic biomass are organisms, like bacteria, who use organic carbon for growth. The autotrophic biomass can be seen as the opposite of heterotrophic biomass. These organisms are able to use sources of energy for the production of organic substrates from inorganic material. Biomass is lost due to decay (e.g. death, predation, lysis). It is assumed that in this case the biomass is transformed into slowly biodegradable substrate (\(X_S\)) and particulate products (\(X_P\)). The last two elements used in ASM1 are dissolved oxygen (\(S_O\)) and the alkalinity of the wastewater, denoted by \(S_{ALK}\). The alkalinity of the water contains information about the pH-value and the ionic charges. In order to compare the components of the Activated Sludge Model No. 1 with the other models a list of the components is given in table 2.4.

All processes in Activated Sludge Model No. 1 depend on certain parameters. These parameters can be found in the matrix of ASM1, where the coefficients and rate equations depend on them. In table 2.5 a list of the parameters is given. The parameters determine for example the amount (and speed) of growth and decay of biomass. Other parameters determine the half-saturation of the corresponding component in the wastewater.

<table>
<thead>
<tr>
<th>Notation</th>
<th>Component</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>(S_{ALK})</td>
<td>Alkalinity of the wastewater</td>
<td>(\text{mol}(\text{HCO}_3^-)L^{-3})</td>
</tr>
<tr>
<td>(S_I)</td>
<td>Soluble inert organic material</td>
<td>(M(COD)L^{-3})</td>
</tr>
<tr>
<td>(S_{ND})</td>
<td>Soluble biodegradable organic nitrogen</td>
<td>(M(N)L^{-3})</td>
</tr>
<tr>
<td>(S_{NH})</td>
<td>Soluble ammonia and ammonium nitrogen</td>
<td>(M(N)L^{-3})</td>
</tr>
<tr>
<td>(S_{NO})</td>
<td>Nitrates and Nitrite nitrogen</td>
<td>(M(N)L^{-3})</td>
</tr>
<tr>
<td>(S_O)</td>
<td>Oxygen</td>
<td>(M(-COD)L^{-3})</td>
</tr>
<tr>
<td>(S_S)</td>
<td>Readily biodegradable substrate</td>
<td>(M(COD)L^{-3})</td>
</tr>
<tr>
<td>(X_{B,A})</td>
<td>Active autotrophic biomass</td>
<td>(M(COD)L^{-3})</td>
</tr>
<tr>
<td>(X_{B,H})</td>
<td>Active heterotrophic biomass</td>
<td>(M(COD)L^{-3})</td>
</tr>
<tr>
<td>(X_I)</td>
<td>Particulate inert organic material</td>
<td>(M(COD)L^{-3})</td>
</tr>
<tr>
<td>(X_{ND})</td>
<td>Particulate biodegradable organic nitrogen</td>
<td>(M(N)L^{-3})</td>
</tr>
<tr>
<td>(X_P)</td>
<td>Particulate products from biomass decay</td>
<td>(M(COD)L^{-3})</td>
</tr>
<tr>
<td>(X_S)</td>
<td>Slowly biodegradable substrate</td>
<td>(M(COD)L^{-3})</td>
</tr>
</tbody>
</table>

Table 2.4: Components of the Activated Sludge Model No. 1. \(M(.)\) denotes the mass in terms of the mentioned material. \(L\) denotes a unit of length (for example metres \(m\)). All terms can thus be seen as a concentration.
2.3. ACTIVATED SLUDGE MODEL NO. 1

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Definition</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Y_A$</td>
<td>Yield of autotrophic biomass</td>
<td>$M(\text{cellCOD})/M(N)$</td>
</tr>
<tr>
<td>$Y_H$</td>
<td>Yield of heterotrophic biomass</td>
<td>$M(\text{cellCOD})/M(COD)$</td>
</tr>
<tr>
<td>$f_p$</td>
<td>Fraction of biomass leading to particulate products</td>
<td></td>
</tr>
<tr>
<td>$iXB$</td>
<td>Mass of nitrogen per mass of COD in biomass</td>
<td>$M(N)/M(COD)$</td>
</tr>
<tr>
<td>$iXP$</td>
<td>Mass of nitrogen per mass of COD in products of biomass</td>
<td>$M(N)/M(COD)$</td>
</tr>
<tr>
<td>$\mu_x$</td>
<td>Maximum specific growth rate for autotrophic and heterotrophic biomass ($x = A, H$ respectively)</td>
<td>day$^{-1}$</td>
</tr>
<tr>
<td>$b_x$</td>
<td>Decay coefficient for autotrophic ($x = A$) and heterotrophic ($x = H$) biomass</td>
<td>day$^{-1}$</td>
</tr>
<tr>
<td>$K_{O,H}$</td>
<td>Oxygen half-saturation coefficient for heterotrophic biomass</td>
<td>$M(O_2)/m^3$</td>
</tr>
<tr>
<td>$K_{O,A}$</td>
<td>Oxygen half-saturation coefficient for autotrophic biomass</td>
<td>$M(O_2)/m^3$</td>
</tr>
<tr>
<td>$K_{NO}$</td>
<td>Nitrate half-saturation coefficient for denitrifying heterotrophic biomass</td>
<td>$M(N)/m^3$</td>
</tr>
<tr>
<td>$K_{NH}$</td>
<td>Ammonia half-saturation coefficient for autotrophic biomass</td>
<td>$M(N)/m^3$</td>
</tr>
<tr>
<td>$K_S$</td>
<td>Half-saturation coefficient for heterotrophic biomass</td>
<td>$M(COD)/m^3$</td>
</tr>
<tr>
<td>$K_X$</td>
<td>Half-saturation coefficient for hydrolysis of slowly biodegradable substrate</td>
<td>$M(COD)/M(\text{cellCOD})$</td>
</tr>
<tr>
<td>$\eta_g$</td>
<td>Correction factor for $\mu_H$ under anoxic conditions</td>
<td></td>
</tr>
<tr>
<td>$\eta_h$</td>
<td>Correction factor for hydrolysis under anoxic conditions</td>
<td></td>
</tr>
<tr>
<td>$k_a$</td>
<td>Maximum specific hydrolysis rate</td>
<td>$M(COD)/(M(\text{cellCOD}) \cdot \text{day})$</td>
</tr>
<tr>
<td>$k_a$</td>
<td>Ammonification rate</td>
<td>$m^3 \cdot \text{COD}/(M \cdot \text{day})$</td>
</tr>
</tbody>
</table>

Table 2.5: List of parameters in Activated Sludge Model No. 1. $M(.)$ denotes the mass (in grams) in terms of the mentioned material.

2.3.2 Processes in ASM1

ASM1 is a model for carbon oxidation, nitrification and denitrification in wastewater treatment plants. The processes in the model can be found in tables 2.2 and 2.3. There are roughly 4 processes, which can be considered. First there is the growth of biomass. This is subdivided in the aerobic growth of heterotrophs, the anoxic growth of heterotrophs and the aerobic growth of autotrophs. The terms aerobic and anoxic give some information about the type of growth and the environment where the growth takes place. Aerobic growth means that the organisms grow in a environment with (dissolved) oxygen. This oxygen is also used for the growth. On the other hand there is the anoxic growth. In this case there is no oxygen in the environment. For the growth of biomass other elements, like nitrate, are used.

Next, we consider the decay of biomass. This is again subdivided into the decay of heterotrophs and the decay of autotrophs. The third process in ASM1 is the ammonification of soluble organic nitrogen. Ammonification is the process where organic nitrogen is converted in ammonia nitrogen. The exact reaction can be found in row 6 of the matrix in table 2.2 and 2.3.

Finally, there is the hydrolysis of particulate material. This is subdivided in hydrolysis
of entrapped organics and the hydrolysis of entrapped organic nitrogen. In AMS 1 hydrolysis are the reactions transforming slowly biodegradable material into readily biodegradable material. It is assumed that the slowly biodegradable material is instantaneously removed from the suspension into the bioflocs (flocs of biomass) in the wastewater. In these bioflocs enzymatic reactions turn it into readily biodegradable material.

One remark about the processes in the model. The processes of carbon oxidation, nitrification and denitrification can not be seen directly in the tables 2.2 and 2.3. These processes are indirectly in the model, for example in the growth and decay of biomass or the ammonification process. These processes use for example the organic substrates in the wastewater for the growth of biomass in the activated sludge. In this way the water is cleaned, because organic material needed for biomass growth is removed from the wastewater.

Activated Sludge Model No.1 is given in matrix notation. To give some insight in the model, this section is concluded with an example equation from the model. Consider the heterotrophic biomass $X_{B,H}$. The biomass is influenced by aerobic growth, anoxic growth and decay. Assume that in the tank the input and output of biomass due to flow are zero. The dynamics of the concentration of heterotrophic biomass is now given by

$$\frac{dX_{B,H}}{dt} = \left( \hat{\mu}_H \frac{S_S}{K_S + S_S} \left[ \frac{S_O}{K_{O,H} + S_O} + \eta_g \frac{S_{O,H}}{K_{O,H} + S_O} \frac{S_{NO}}{S_{NO} + K_{NO}} \right] - b_H \right) X_{B,H}. \quad (2.9)$$

### 2.3.3 Limitations of ASM1

Since AMS1 is a simple model of the real wastewater treatment plants there are some limitations (see for example [8,14]). First of all the system operates at a constant temperature and pH, which is near neutral. The model is developed for municipal wastewater only, industrial wastewater can not be modelled with ASM1. Also the parameter values in the rate equations are assumed to be constant. The coefficients for the nitrification process are assumed to be constant. Also the correction factors of denitrification ($\eta_g$ and $\eta_h$) are constants in the model.

Furthermore it is assumed that the heterotrophic biomass is homogeneous and does not change in species diversity. The entrapment of particulate organic material is assumed to be instantaneous. Also the hydrolysis of organic matter and organic nitrogen occur simultaneously in the model, with equal reaction rates. Finally the type of electron acceptor is assumed not to affect the loss of biomass by decay.

In using ASM1, there are also a few restrictions. The net growth rate of the biomass must be within a range that allows a development of flocculent biomass. Flocculent biomass is the result of a flocculation process. In this process particles in a suspension stick together and form flocs. So flocculent biomass is biomass in the form of flocs.

The unaerated fraction of the reactor volume in the model may not exceed 50%, otherwise the sludge settling (sludge sticks to the wall of a tank) characteristics may become worse. This limitation is mentioned in [8]. There is no hard evidence mentioned why this...
fraction may not exceed 50%. Personally, I think this limitation is weak, and is probably observed by doing some experiments.

2.4 Activated Sludge Model No. 2

Activated Sludge Model No. 2 is the successor of ASM1. Where ASM1 modelled the combined biological processes for Chemical Oxygen Demand and nitrogen removal, ASM2 adds the biological process for phosphorus removal to the model. It was introduced in 1995 by the task group of the IAWQ [7].

The model is again a tool for research, teaching, process optimization in existing wastewater treatment plants and the design of WWTPs. The model is a compromise between complexity and simplicity. For example, the kinetics and stoichiometry are chosen as simply as possible, just as in ASM1. One of the major differences between both models is that biomass now has a cell internal structure. This means that some elements in the wastewater may be stored in the cell of an organism. In ASM1 it is assumed that this is not possible. This also means that the concentration cannot be described by $X_{B,H}$ and $X_{B,A}$. An additional component for the storage of material in a cell is needed. ASM2 can be simplified by eliminating those components, which do not have a dominant effect upon the kinetics of the processes, or the performance.

2.4.1 Components in ASM2

In this section all components of ASM2 are considered. Again, $S_i$ means a soluble element and $X_i$ means a particulate element. Furthermore, all particulate material is assumed to be neutral, whereas soluble material may carry ionic charges. Also all components are assumed to be homogeneous and completely distributed through the system of interest. In table 2.6 all components of ASM2 can be found.

Just like Activated Sludge Model No.1, ASM2 consists out of many parameters defining the amount and speed of growth and decay of biomass. But also the yield of some components and different fractions and ratios between the components. A complete list, together with typical values can be found in [7]. In table 2.7 only a short summary of the notation is given.
<table>
<thead>
<tr>
<th>Notation</th>
<th>Component</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S_A$</td>
<td>Fermentation products, acetate</td>
<td>$M(COD)L^{-3}$</td>
</tr>
<tr>
<td>$S_{ALK}$</td>
<td>Alkalinity of wastewater</td>
<td>$mol(HCO_3^-)L^{-3}$</td>
</tr>
<tr>
<td>$S_F$</td>
<td>Fermentable, readily biodegradable organic substrate</td>
<td>$M(COD)L^{-3}$</td>
</tr>
<tr>
<td>$S_I$</td>
<td>Inert soluble organic material</td>
<td>$M(COD)L^{-3}$</td>
</tr>
<tr>
<td>$S_{N_2}$</td>
<td>Dinitrogen, $N_2$</td>
<td>$M(N)L^{-3}$</td>
</tr>
<tr>
<td>$S_{NH_4}$</td>
<td>Ammonium and ammonia nitrogen</td>
<td>$M(N)L^{-3}$</td>
</tr>
<tr>
<td>$S_{NO_3}$</td>
<td>Nitrate and nitrite nitrogen</td>
<td>$M(N)L^{-3}$</td>
</tr>
<tr>
<td>$S_{O_2}$</td>
<td>Dissolved oxygen</td>
<td>$M(O_2)L^{-3}$</td>
</tr>
<tr>
<td>$S_{PO_4}$</td>
<td>Inorganic soluble phosphorus, primarily ortho-phosphates</td>
<td>$M(P)L^{-3}$</td>
</tr>
<tr>
<td>$S_S$</td>
<td>Readily biodegradable substrate, $S_F + S_A$</td>
<td>$M(COD)L^{-3}$</td>
</tr>
<tr>
<td>$X_{AUT}$</td>
<td>Nitrifying organisms</td>
<td>$M(COD)L^{-3}$</td>
</tr>
<tr>
<td>$X_H$</td>
<td>Heterotrophic organisms</td>
<td>$M(COD)L^{-3}$</td>
</tr>
<tr>
<td>$X_I$</td>
<td>Inert particulate material</td>
<td>$M(COD)L^{-3}$</td>
</tr>
<tr>
<td>$X_{MeOH}$</td>
<td>Metal-hydroxides, $Me =$ some metal (for example Fe)</td>
<td>$M(TSS)L^{-3}$</td>
</tr>
<tr>
<td>$X_{MeP}$</td>
<td>Metal-phosphate, $MePO_4$</td>
<td>$M(TSS)L^{-3}$</td>
</tr>
<tr>
<td>$X_{PAO}$</td>
<td>Phosphate accumulating organisms (PAO)</td>
<td>$M(COD)L^{-3}$</td>
</tr>
<tr>
<td>$X_{PHA}$</td>
<td>Cell internal storage product of PAO</td>
<td>$M(COD)L^{-3}$</td>
</tr>
<tr>
<td>$X_{PP}$</td>
<td>Poly-phosphate</td>
<td>$M(P)L^{-3}$</td>
</tr>
<tr>
<td>$X_S$</td>
<td>Slowly biodegradable substrates</td>
<td>$M(COD)L^{-3}$</td>
</tr>
<tr>
<td>$X_{TSS}$</td>
<td>Total suspended solids</td>
<td>$M(TSS)L^{-3}$</td>
</tr>
</tbody>
</table>

Table 2.6: Components of the Activated Sludge Model No. 2. $M(.)$ denotes the mass in terms of the mentioned material. $L$ denotes a unit of length (for example metres $m$). All terms can thus be seen as a concentration.
### 2.4. Activated Sludge Model No. 2

<table>
<thead>
<tr>
<th>Notation</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$i_x$</td>
<td>Conversion factor defining the content of a certain component of another component in the model. For example: $i_{NS_I}$ is $N$ content of $S_I$. Concentration of $N$ in $S_I$.</td>
</tr>
<tr>
<td>$f_x$</td>
<td>Fraction of material. $x$ shows what components. For example:</td>
</tr>
<tr>
<td>$Y_x$</td>
<td>Yield coefficient. Again $x$ is a component in the model.</td>
</tr>
<tr>
<td>$K_x$</td>
<td>Saturation coefficient for the corresponding component.</td>
</tr>
<tr>
<td>$\eta_x$</td>
<td>Correction factor for growth.</td>
</tr>
<tr>
<td>$\mu_x$</td>
<td>Maximum growth rate. $x$ is the component.</td>
</tr>
<tr>
<td>$b_x$</td>
<td>Rate constant for lysis (decay rate). Again $x$ shows the component.</td>
</tr>
<tr>
<td>$k_x$</td>
<td>Rate constant.</td>
</tr>
<tr>
<td>$q_x$</td>
<td>Rate constant.</td>
</tr>
</tbody>
</table>

Table 2.7: Notation of the different parameters in Activated Sludge Model No. 2. A complete list can be found in [7].

ASM2 is introduced using the same matrix notation as ASM1. So the following notation is used:

- index $i$, the components in the model, row in the matrix,
- index $j$, the processes in the model, column in the matrix,
- $\nu_{ij}$, the stoichiometric matrix elements,
- $\rho_{ij}$, the process rate equations.

Again the production rate for the reaction term in the mass-balance is given by equation 2.3. The corresponding matrix for ASM2 is too large to present in one table. Therefore the matrix is given in a few smaller tables. These are treated in the next section. In ASM2 the stoichiometry is based on the continuity equations. For COD, electrical charges and nitrogen this can be compared with ASM1. ASM2 adds continuity equations for phosphorus and an equation transforming the unit of measurement of the solid components into total suspended solids.

#### 2.4.2 Processes in ASM2

The descriptions of the biological processes of the Activated Sludge Model No. 2 are based on the average behaviour of the different micro-organisms. As stated above ASM2 is not given in one large matrix, but in a few smaller tables. These tables could be combined into one large matrix representing the complete AMS2 model. In table 2.8 all rate equations of ASM2 can be found. All processes are treated individually, in smaller tables. All tables together represent the matrix notation as we have seen for Activated Sludge Model No. 1.
<table>
<thead>
<tr>
<th>Process</th>
<th>Rate equation $\rho_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrolysis processes</td>
<td>$K_h \frac{S_{O_2}}{K_{O_2} + S_{O_2}} \frac{X_B}{K_x + S_x/A_H} X_B$</td>
</tr>
<tr>
<td>1. Aerobic hydrolysis</td>
<td>$K_h \bullet q_{P} \frac{S_{O_2}}{K_{O_2} + S_{O_2}} \frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}} \frac{X_B}{K_x + S_x/A_H} X_B$</td>
</tr>
<tr>
<td>2. Anoxic hydrolysis</td>
<td>$K_h \bullet q_{P} \frac{X_B}{K_x + S_x/A_H} X_B$</td>
</tr>
<tr>
<td>3. Anaerobic hydrolysis</td>
<td>$K_h \bullet q_{P} \frac{X_B}{K_x + S_x/A_H} X_B$</td>
</tr>
<tr>
<td>Heterotrophic organisms</td>
<td>$\rho_H = \frac{S_{O_2}}{K_{O_2} + S_{O_2}}$</td>
</tr>
<tr>
<td>4. Growth on $S_P$</td>
<td>$\rho_H = \frac{S_{P}}{K_{P} + S_{P}}$</td>
</tr>
<tr>
<td>5. Growth on $S_A$</td>
<td>$\rho_H = \frac{S_{A}}{K_{A} + S_{A}}$</td>
</tr>
<tr>
<td>6. Denitrification on $S_P$</td>
<td>$\rho_H = \frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}} \frac{S_{P}}{K_{P} + S_{P}}$</td>
</tr>
<tr>
<td>7. Denitrification on $S_A$</td>
<td>$\rho_H = \frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}} \frac{S_{A}}{K_{A} + S_{A}}$</td>
</tr>
<tr>
<td>8. Fermentation</td>
<td>$\rho_H = \frac{S_{P}}{K_{P} + S_{P}}$</td>
</tr>
<tr>
<td>9. Lysis</td>
<td>$\rho_H = \frac{S_{A}}{K_{A} + S_{A}}$</td>
</tr>
<tr>
<td>Phosphorus-accumulation organisms</td>
<td>$\rho_{PHA} = \frac{S_{P}}{K_{P} + S_{P}}$</td>
</tr>
<tr>
<td>10. Storage of $X_{PHA}$</td>
<td>$\rho_{PHA} = \frac{S_{P}}{K_{P} + S_{P}}$</td>
</tr>
<tr>
<td>11. Storage of $X_{PP}$</td>
<td>$\rho_{PHA} = \frac{S_{P}}{K_{P} + S_{P}}$</td>
</tr>
<tr>
<td>12. Aerobic growth on $X_{PHA}$</td>
<td>$\rho_{PHA} = \frac{S_{P}}{K_{P} + S_{P}}$</td>
</tr>
<tr>
<td>13. Lysis of $X_{PHA}$</td>
<td>$\rho_{PHA} = \frac{S_{P}}{K_{P} + S_{P}}$</td>
</tr>
<tr>
<td>14. Lysis of $X_{PP}$</td>
<td>$\rho_{PHA} = \frac{S_{P}}{K_{P} + S_{P}}$</td>
</tr>
<tr>
<td>15. Lysis of $X_{PP}$</td>
<td>$\rho_{PHA} = \frac{S_{P}}{K_{P} + S_{P}}$</td>
</tr>
<tr>
<td>Nitrifying organisms</td>
<td>$\rho_{AUT} = \frac{S_{NO_2}}{K_{NO_2} + S_{NO_2}}$</td>
</tr>
<tr>
<td>16. Growth</td>
<td>$\rho_{AUT} = \frac{S_{NO_2}}{K_{NO_2} + S_{NO_2}}$</td>
</tr>
<tr>
<td>17. Lysis</td>
<td>$\rho_{AUT} = \frac{S_{NO_2}}{K_{NO_2} + S_{NO_2}}$</td>
</tr>
<tr>
<td>Precipitation of phosphorus</td>
<td>$k_{PRE} \cdot S_{PO_4} \cdot X_{MgOH}$</td>
</tr>
<tr>
<td>18. Precipitation</td>
<td>$k_{PRE} \cdot S_{PO_4} \cdot X_{MgOH}$</td>
</tr>
<tr>
<td>19. Redissolution</td>
<td>$k_{RED} \cdot X_{MgOH} \cdot S_{ALK}$</td>
</tr>
</tbody>
</table>

Table 2.8: Rate equations of Activated Sludge model No. 2.

First we consider the hydrolysis processes, the enzymatic reactions by a cell. There are three types of processes. First, aerobic hydrolysis of slowly biodegradable substrate, which characterizes the hydrolysis under aerobic conditions, so $S_{O_2} > 0$. Then there is anoxic hydrolysis, where the anoxic conditions $S_{O_2} \approx 0$ and $S_{NO_3} > 0$ hold. Finally there is anaerobic hydrolysis. This is the hydrolysis of slowly biodegradable substrate under the conditions that $S_{O_2} \approx 0$ and $S_{NO_3} \approx 0$. Anaerobic means that there is no oxygen at all in the environment. It also means that no oxygen is used in this process. The rate of this process is probably slower than aerobic hydrolysis. In Table 2.9 these processes can be found together with the stoichiometric parameters.
2.4. ACTIVATED SLUDGE MODEL NO. 2

Table 2.9: Stoichiometric coefficients of the hydrolysis processes.

<table>
<thead>
<tr>
<th>j</th>
<th>Process</th>
<th>( S_F )</th>
<th>( S_{NH_4} )</th>
<th>( S_{PO_4} )</th>
<th>( S_I )</th>
<th>( S_{ALK} )</th>
<th>( X_S )</th>
<th>( X_{TSS} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Aerobic hydrolysis</td>
<td>( 1 - f_{S_I} ) ( \nu_{1,NH_4} ) ( \nu_{1,PO_4} )</td>
<td>( f_{S_I} ) ( \nu_{1,ALK} )</td>
<td>-1</td>
<td>( \nu_{1,TSS} )</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>Anoxic hydrolysis</td>
<td>( 1 - f_{S_I} ) ( \nu_{2,NH_4} ) ( \nu_{2,PO_4} )</td>
<td>( f_{S_I} ) ( \nu_{2,ALK} )</td>
<td>-1</td>
<td>( \nu_{2,TSS} )</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>Anaerobic hydrolysis</td>
<td>( 1 - f_{S_I} ) ( \nu_{3,NH_4} ) ( \nu_{3,PO_4} )</td>
<td>( f_{S_I} ) ( \nu_{3,ALK} )</td>
<td>-1</td>
<td>( \nu_{3,TSS} )</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Next the processes of heterotrophic organisms are treated. The processes, with their stoichiometric coefficients can be found in table 2.10. Again the corresponding rate equations are in table 2.8. It contains the aerobic growth of heterotrophic organisms and the anoxic growth of organisms (denitrification). Also fermentation and lysis of heterotrophic organisms are in ASM2. Fermentation is the process of energy production in a cell under anaerobic conditions, so without any oxygen. The energy is released by the oxidation of organic material, using a cell internal electron acceptor.

Table 2.10: Stoichiometric coefficients of the growth and decay of heterotrophic organisms. \( Y_H \) is a fixed yield coefficient.

<table>
<thead>
<tr>
<th>j</th>
<th>Process</th>
<th>( S_{O_2} )</th>
<th>( S_F )</th>
<th>( S_A )</th>
<th>( S_{NO_3} )</th>
<th>( S_{N_2} )</th>
<th>( X_I )</th>
<th>( X_S )</th>
<th>( X_H )</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>Aerobic growth on ( S_F )</td>
<td>1</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>1</td>
<td>( \frac{1}{Y_H} )</td>
<td>1</td>
</tr>
<tr>
<td>5</td>
<td>Aerobic growth on ( S_A )</td>
<td>1</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>1</td>
<td>( \frac{1}{Y_H} )</td>
<td>1</td>
</tr>
<tr>
<td>6</td>
<td>Anoxic growth on ( S_F )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>Anoxic growth on ( S_A )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>Fermentation</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>Lysis</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td></td>
</tr>
</tbody>
</table>

Table 2.11: Stoichiometric coefficients of the processes of phosphorus accumulating organisms.

<table>
<thead>
<tr>
<th>j</th>
<th>Process</th>
<th>( S_{O_2} )</th>
<th>( S_A )</th>
<th>( S_{PO_4} )</th>
<th>( X_I )</th>
<th>( X_S )</th>
<th>( X_{PO_A} )</th>
<th>( X_{PP} )</th>
<th>( X_{PHA} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>Storage of ( X_{PHA} )</td>
<td>( -1 )</td>
<td>( Y_{PO_4} )</td>
<td>( -1 )</td>
<td>( Y_{PO_4} )</td>
<td>( -1 )</td>
<td>( Y_{PHA} )</td>
<td>( -1 )</td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>Storage of ( X_{PP} )</td>
<td>( -Y_{PHA} )</td>
<td>( -1 )</td>
<td>( -1 )</td>
<td>( -1 )</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>Aerobic growth</td>
<td>( \frac{1}{Y_H} )</td>
<td>( -i_{PBM} )</td>
<td>( f_{X_I} )</td>
<td>( 1 - f_{X_I} )</td>
<td>1</td>
<td>( -1 )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>Lysis of ( X_{PAO} )</td>
<td>( -1 )</td>
<td>( \nu_{3,P} )</td>
<td>( f_{X_I} )</td>
<td>( 1 - f_{X_I} )</td>
<td>-1</td>
<td>( -1 )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>Lysis of ( X_{PP} )</td>
<td>( 1 )</td>
<td>( -1 )</td>
<td>( 1 )</td>
<td>( -1 )</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>Lysis of ( X_{PHA} )</td>
<td>( 1 )</td>
<td>( -1 )</td>
<td>( 1 )</td>
<td>( -1 )</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

New in the activated sludge model is the treatment of phosphorus removal. One of the processes involved is the storage of phosphorus accumulating organisms and polyphosphate. Other processes are the aerobic growth and lysis of phosphorus accumulating organisms, the lysis of poly-phosphate and internal cell storage of the products of PAOs. The stoichiometric coefficients for these processes can be found in table 2.11. while the rate equations are again in table 2.8.
Another process in ASM2 is the aerobic growth of nitrifying organisms. Together with the lysis of nitrifying organisms the stoichiometry can be found in table 2.12.

<table>
<thead>
<tr>
<th>$j$</th>
<th>Process</th>
<th>$S_{O_2}$</th>
<th>$S_{NH_4}$</th>
<th>$S_{NO_3}$</th>
<th>$S_{PO_4}$</th>
<th>$X_I$</th>
<th>$X_S$</th>
<th>$X_{AUT}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>Aerobic growth of $X_{AUT}$</td>
<td>$-\frac{4.57 - Y_A}{Y_A}$</td>
<td>$-i_{NBM} \frac{1}{Y_A}$</td>
<td>$\frac{1}{Y_A}$</td>
<td>$-i_{PBM}$</td>
<td>$\nu_{17,NH_4}$</td>
<td>$\nu_{17,PO_4}$</td>
<td>$f_{X_I}$</td>
</tr>
<tr>
<td>17</td>
<td>Lysis</td>
<td>$\nu_{17,NH_4}$</td>
<td>$\nu_{17,PO_4}$</td>
<td>$f_{X_I}$</td>
<td>$1 - f_{X_I}$</td>
<td>1</td>
<td>-1</td>
<td></td>
</tr>
</tbody>
</table>

Table 2.12: Stoichiometric coefficients of the nitrification processes.

The last two processes in the model are the chemical precipitation and redissolution of phosphate. Again the stoichiometry can be found in a table, table 2.13 and the rate equations in table 2.8. Chemical precipitation is a process where a solid material is formed in a solution. This formation can be due to a chemical reaction or by diffusion. In AMS 2 redissolution is assumed to be the opposite process of precipitation. In a steady state situation this would lead to an equilibrium.

<table>
<thead>
<tr>
<th>$j$</th>
<th>Process</th>
<th>$S_{PO_4}$</th>
<th>$S_{ALK}$</th>
<th>$X_{MeOH}$</th>
<th>$X_{MeP}$</th>
<th>$X_{TSS}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>18</td>
<td>Precipitation</td>
<td>-1</td>
<td>$\nu_{19,ALK}$</td>
<td>-3.45</td>
<td>4.87</td>
<td>1.42</td>
</tr>
<tr>
<td>19</td>
<td>Redissolution</td>
<td>1</td>
<td>$\nu_{20,ALK}$</td>
<td>3.45</td>
<td>-4.87</td>
<td>-1.42</td>
</tr>
</tbody>
</table>

Table 2.13: Stoichiometric coefficients of the processes describing simultaneous precipitation and redissolution of phosphorus. The values in this table are based on the assumption that the metal $Me$ is Ferro (Fe).

### 2.4.3 Limitations of ASM2

The Activated Sludge Model No. 2 has the same assumptions and restrictions as Activated Sludge Model No. 1. This is due to the fact that ASM2 is based on ASM1, certain processes are more or less the same in both models. It also means that a lot of values in ASM2, like temperature, pH, coefficients in rate equations are assumed to be constant, just as in ASM1. But there are also some extended assumptions. It is assumed that the heterotrophic biomass and the phosphorus accumulating biomass are homogeneous. The biomass does not changes in time. It also assumed that the hydrolysis of organic matter, organic nitrogen and organic phosphorus are coupled and occur simultaneously.

Next to above assumptions there are some new assumptions in ASM2 on phosphate accumulating organisms. The fermentation products are assumed to be the only organic substrates that can be taken up by the PAO (Phosphorus Accumulating Organisms). Also the PAO can grow aerobically only on stored PHA (Poly-Hydroxy-Alkanoates), which represents all carbon storage materials in PAO cells. Furthermore it is assumed that the PAO do not have any denitrifying capability. Also, the model does not contain separate
biomass for the fraction of heterotrophs that store PHA. And, finally, the heterotrophs are assumed to grow aerobically, denitrify anoxically and ferment anaerobically.

ASM2 does have some restrictions due to the structure of the model. It can only deal with low phosphate and ammonia concentrations. The fractions of organic substrates are assumed to be homogeneous and their nature should not change at all. Limitations of the metals potassium and magnesium are not considered in the biological phosphorus removal. Just like the influence of $NO_2^-$ and $NO_3^-$ on the removal process.

Just like ASM1, ASM2 is only suitable for domestic wastewater. The value of pH should be near neutrality, so takes a value between 6.3 and 7.8. Finally, the temperature must be limited to 10-25°C. This may look like a contradiction with the assumption that the temperature and pH must be constant. Using the model requires constant values for both, but for a different temperature and pH, all parameters are slightly different. The model is only valid for constant values chosen within the mentioned range of temperature and pH.

2.5 Activated Sludge Model No. 2d

The third activated sludge model introduced by the IAWQ task group is the Activated Sludge Model No. 2d. The model is a minor extension of ASM2, including two additional processes modelling phosphate accumulating organisms (PAO), which use internal organic storage products for denitrification. All remarks and limitations of ASM2 are also valid for ASM2d.

2.5.1 Components in AMS2d

The components in ASM2d are the same as in ASM2. In table 2.6 these components can be found. Also the parameters in the model are the same. The soluble material may carry ionic charges. The particulate material is assumed to be associated with the activated sludge (floculated) and must be electrically neutral. Furthermore, all components are assumed to be homogeneous and distributed throughout the system of interest.

Just as ASM1 and ASM2, the task group introduces ASM2d using the previously explained matrix notation. The same notation is used here. Conservation equations in the model are the mathematical equivalent of the principles of chemical reactions, chemical elements and electrons.

2.5.2 Processes in ASM2d

As said before, ASM2d is a minor extension of ASM2. Most processes are introduced in ASM2 and are the same in ASM2d. Micro-organisms in an activated sludge system have a complex internal cell structure. They also respond to different environmental conditions by adjusting this internal structure. ASM2 is a model where each biological process represents a large number of ‘sub’-processes acting on a variety of substances in the wastewater.
The rate equations for ASM2d can be found in table 2.14. Also the rate equations are the same, they are made with hyperbolic switching functions. The rate equations for ASM2d can be found in table 2.14.

<table>
<thead>
<tr>
<th>Process</th>
<th>Rate equation $r_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Hydrolysis processes</strong></td>
<td></td>
</tr>
<tr>
<td>1. Aerobic hydrolysis</td>
<td>$\mu_b \frac{SO_2}{NO_2 + SO_2} X_H$</td>
</tr>
<tr>
<td>2. Anoxic hydrolysis</td>
<td>$\eta NO_2 \frac{SO_2}{NO_2 + SO_2}$</td>
</tr>
<tr>
<td>3. Anaerobic hydrolysis</td>
<td>$\eta fe \frac{SO_2}{NO_2 + SO_2}$</td>
</tr>
<tr>
<td><strong>Heterotrophic organisms</strong></td>
<td></td>
</tr>
<tr>
<td>4. Growth on $S_F$</td>
<td>$\mu_H \frac{SO_2}{NO_2 + SO_2}$</td>
</tr>
<tr>
<td>5. Growth on $S_A$</td>
<td>$\mu_H \frac{SO_2}{NO_2 + SO_2}$</td>
</tr>
<tr>
<td>6. Denitrification on $S_F$</td>
<td>$\eta NO_2 \frac{SO_2}{NO_2 + SO_2}$</td>
</tr>
<tr>
<td>7. Denitrification on $S_A$</td>
<td>$\eta NO_2 \frac{SO_2}{NO_2 + SO_2}$</td>
</tr>
<tr>
<td>8. Fermentation</td>
<td>$\eta fe \frac{K_O}{NO_2 + SO_2}$</td>
</tr>
<tr>
<td>9. Lysis</td>
<td>$\eta H \frac{X_H}{X_H}$</td>
</tr>
<tr>
<td><strong>Phosphorus accumulation organisms</strong></td>
<td></td>
</tr>
<tr>
<td>10. Storage of $X_{PAO}$</td>
<td>$q_{PHA} \frac{SA}{KA + SA}$</td>
</tr>
<tr>
<td>11. Aerobic storage of $X_{PAO}$</td>
<td>$q_{PP} \frac{SO_2}{NO_2 + SO_2}$</td>
</tr>
<tr>
<td>12. Anoxic storage of $X_{PAO}$</td>
<td>$q_{PAO} \frac{SO_2}{NO_2 + SO_2}$</td>
</tr>
<tr>
<td>13. Aerobic growth on $X_{PHA}$</td>
<td>$\rho_{11} \frac{\eta NO_2}{SO_2}$</td>
</tr>
<tr>
<td>14. Anoxic growth on $X_{PHA}$</td>
<td>$\rho_{13} \frac{\eta NO_2}{SO_2}$</td>
</tr>
<tr>
<td>15. Lysis of $X_{PAO}$</td>
<td>$b_{PAO} \cdot X_{PAO} \frac{SA}{ALK + ALK}$</td>
</tr>
<tr>
<td>16. Lysis of $X_{PP}$</td>
<td>$b_{PP} \cdot X_{PP} \frac{SA}{ALK + ALK}$</td>
</tr>
<tr>
<td>17. Lysis of $X_{PHA}$</td>
<td>$b_{PHA} \cdot X_{PHA} \frac{SA}{ALK + ALK}$</td>
</tr>
<tr>
<td><strong>Nitrifying organisms</strong></td>
<td></td>
</tr>
<tr>
<td>18. Growth</td>
<td>$\mu_{AUT} \frac{SO_2}{NO_2 + SO_2}$</td>
</tr>
<tr>
<td>19. Lysis</td>
<td>$\eta_{AUT} \frac{X_{AUT}}{X_{AUT}}$</td>
</tr>
<tr>
<td><strong>Precipitation of phosphorus</strong></td>
<td></td>
</tr>
<tr>
<td>20. Precipitation</td>
<td>$k_{PRE} \cdot SO_4 \cdot XM_\text{M} \cdot \frac{SA}{ALK + ALK}$</td>
</tr>
<tr>
<td>21. Redissolution</td>
<td>$k_{RED} \cdot XM_\text{M} \cdot \frac{SA}{ALK + ALK}$</td>
</tr>
</tbody>
</table>

Table 2.14: Rate equations of Activated Sludge model No. 2d.

The processes of heterotrophic organisms are almost the same in ASM2d, compared with ASM2. In the stoichiometric coefficients there is an additional minus sign for anoxic growth (see table 2.16).
2.5. Activated Sludge Model No. 2D

<table>
<thead>
<tr>
<th>j</th>
<th>Process</th>
<th>( S_F )</th>
<th>( S_{NH_4} )</th>
<th>( S_{PO_4} )</th>
<th>( S_L )</th>
<th>( S_{ALK} )</th>
<th>( X_S )</th>
<th>( X_{TSS} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Aerobic hydrolysis</td>
<td>( 1 - f_S )</td>
<td>( \nu_1, NH_4 )</td>
<td>( \nu_1, PO_4 )</td>
<td>( \bar{s_I} )</td>
<td>( \nu_1, ALK )</td>
<td>-1</td>
<td>( \nu_1, TSS )</td>
</tr>
<tr>
<td>2</td>
<td>Anoxic hydrolysis</td>
<td>( 1 - f_S )</td>
<td>( \nu_2, NH_4 )</td>
<td>( \nu_2, PO_4 )</td>
<td>( \bar{s_I} )</td>
<td>( \nu_2, ALK )</td>
<td>-1</td>
<td>( \nu_2, TSS )</td>
</tr>
<tr>
<td>3</td>
<td>Anaerobic hydrolysis</td>
<td>( 1 - f_S )</td>
<td>( \nu_3, NH_4 )</td>
<td>( \nu_3, PO_4 )</td>
<td>( \bar{s_I} )</td>
<td>( \nu_3, ALK )</td>
<td>-1</td>
<td>( \nu_3, TSS )</td>
</tr>
</tbody>
</table>

Table 2.15: Stoichiometric coefficients of the hydrolysis processes.

<table>
<thead>
<tr>
<th>j</th>
<th>Process</th>
<th>( S_{O_2} )</th>
<th>( S_F )</th>
<th>( S_A )</th>
<th>( S_{NO_3} )</th>
<th>( S_{N_2} )</th>
<th>( X_I )</th>
<th>( X_S )</th>
<th>( X_H )</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>Aerobic growth on ( S_F )</td>
<td>( 1 - \frac{Y_P O_4}{Y_H} )</td>
<td>( -\frac{1}{Y_H} )</td>
<td>( \bar{s_I} )</td>
<td>( \nu_1, PO_4 )</td>
<td>( \nu_1, ALK )</td>
<td>( \bar{s_I} )</td>
<td>( \nu_1, TSS )</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>Aerobic growth on ( S_A )</td>
<td>( 1 - \frac{Y_P O_4}{Y_H} )</td>
<td>( -\frac{1}{Y_H} )</td>
<td>( \bar{s_I} )</td>
<td>( \nu_1, PO_4 )</td>
<td>( \nu_1, ALK )</td>
<td>( \bar{s_I} )</td>
<td>( \nu_1, TSS )</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>Anoxic growth on ( S_F )</td>
<td>( -\frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>Anoxic growth on ( S_A )</td>
<td>( 1 )</td>
<td>( -\frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>Fermentation</td>
<td>( -1 )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>Lysis</td>
<td>( f_X_I )</td>
<td>( 1 - f_X_I )</td>
<td>( -1 )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td>( \frac{1}{Y_H} )</td>
<td></td>
</tr>
</tbody>
</table>

Table 2.16: Stoichiometric coefficients of the growth and decay of heterotrophic organisms. \( Y_H \) is the yield coefficient.

If we look at the processes of phosphorus accumulating organisms then we see in ASM2d two additional processes compared with ASM2. The model also takes into account that PAOs can denitrify. Phosphate release is in fact slower in the presence of nitrate. In the model the storage of poly-phosphates is split into the aerobic and anoxic storage of \( X_{PP} \). Also the growth of PAOs is split into aerobic and anoxic. In table 2.14 we see two additional rate equations. In table 2.17 all stoichiometric coefficients can be found.

<table>
<thead>
<tr>
<th>j</th>
<th>Process</th>
<th>( S_{O_2} )</th>
<th>( S_A )</th>
<th>( S_{NO_3} )</th>
<th>( S_{PO_4} )</th>
<th>( X_I )</th>
<th>( X_S )</th>
<th>( X_PAO )</th>
<th>( X_{PP} )</th>
<th>( X_{PHA} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>Storage of ( X_{PHA} )</td>
<td>( -1 )</td>
<td>( \bar{s_I} )</td>
<td>( \nu_1, PO_4 )</td>
<td>( \bar{s_I} )</td>
<td>( \nu_1, ALK )</td>
<td>( \bar{s_I} )</td>
<td>( \nu_1, TSS )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>Aerobic storage of ( X_{PP} )</td>
<td>( -Y_{PHA} )</td>
<td>( -1 )</td>
<td>( \nu_1, PO_4 )</td>
<td>( \bar{s_I} )</td>
<td>( \nu_1, ALK )</td>
<td>( \bar{s_I} )</td>
<td>( \nu_1, TSS )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>Anoxic storage of ( X_{PP} )</td>
<td>( -\nu_1, NO_3 )</td>
<td>( \nu_1, PO_4 )</td>
<td>( \bar{s_I} )</td>
<td>( \nu_1, ALK )</td>
<td>( \bar{s_I} )</td>
<td>( \nu_1, TSS )</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>Aerobic growth of ( X_{PANO} )</td>
<td>( \nu_1, O_2 )</td>
<td>( -i_{PB} )</td>
<td>( \bar{s_I} )</td>
<td>( \nu_1, PO_4 )</td>
<td>( \bar{s_I} )</td>
<td>( \nu_1, TSS )</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>Anoxic growth of ( X_{PANO} )</td>
<td>( -\nu_1, NO_3 )</td>
<td>( \nu_1, PO_4 )</td>
<td>( \bar{s_I} )</td>
<td>( \nu_1, ALK )</td>
<td>( \bar{s_I} )</td>
<td>( \nu_1, TSS )</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>Lysis of ( X_{PPO} )</td>
<td>( -\nu_1, PO_4 )</td>
<td>( \bar{s_I} )</td>
<td>( \nu_1, ALK )</td>
<td>( \bar{s_I} )</td>
<td>( \nu_1, TSS )</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>Lysis of ( X_{PP} )</td>
<td>( 1 )</td>
<td>( -1 )</td>
<td>( \nu_1, TSS )</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>17</td>
<td>Lysis of ( X_{PHA} )</td>
<td>( 1 )</td>
<td>( -1 )</td>
<td>( \nu_1, TSS )</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 2.17: Stoichiometric coefficients of the processes of phosphorus accumulating organisms.
In ASM2d the nitrification processes are assumed to be an one-step-process. So in the model $S_{NH_4}$ transforms immediately into $S_{NO_3}$. The nitrite in between this transformation is not in the model available. Again the stoichiometric coefficients can be found in table 2.18 and the rate equations are in table 2.14.

<table>
<thead>
<tr>
<th>( j )</th>
<th>Process</th>
<th>( S_{O_2} )</th>
<th>( S_{NH_4} )</th>
<th>( S_{NO_3} )</th>
<th>( S_{PO_4} )</th>
<th>( X_I )</th>
<th>( X_S )</th>
<th>( X_{AUT} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>18</td>
<td>Aerobic growth of ( X_{AUT} )</td>
<td>( -\frac{3.97-3.57}{Y_A} ) ( v_{18,NH_4} )</td>
<td>( 1 ) ( v_{18,NH_4} )</td>
<td>( 1 ) ( v_{18,NH_4} )</td>
<td>( 1 ) ( v_{18,NH_4} )</td>
<td>( 1 ) ( v_{18,NH_4} )</td>
<td>( 1 ) ( v_{18,NH_4} )</td>
<td>( 1 ) ( v_{18,NH_4} )</td>
</tr>
<tr>
<td>19</td>
<td>Lysis</td>
<td>( 1 ) ( v_{19,NH_4} )</td>
<td>( 1 ) ( v_{19,NH_4} )</td>
<td>( 1 ) ( v_{19,NH_4} )</td>
<td>( 1 ) ( v_{19,NH_4} )</td>
<td>( 1 ) ( v_{19,NH_4} )</td>
<td>( 1 ) ( v_{19,NH_4} )</td>
<td>( 1 ) ( v_{19,NH_4} )</td>
</tr>
</tbody>
</table>

Table 2.18: Stoichiometric coefficients of the nitrification processes.

Just as in ASM2, the last processes in ASM2 are the chemical precipitation and redissolution. Again these processes are assumed to act simultaneously. The stoichiometry can be found in table 2.19. It is assumed that the metal in these processes is ferro.

<table>
<thead>
<tr>
<th>( j )</th>
<th>Process</th>
<th>( S_{PO_4} )</th>
<th>( S_{ALK} )</th>
<th>( X_{MeOH} )</th>
<th>( X_{MeP} )</th>
<th>( X_{TSS} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>Precipitation</td>
<td>( -1 ) ( v_{20,ALK} )</td>
<td>( -3.45 ) ( v_{20,ALK} )</td>
<td>( 1.42 ) ( v_{20,ALK} )</td>
<td>( 1.42 ) ( v_{20,ALK} )</td>
<td>( 1.42 ) ( v_{20,ALK} )</td>
</tr>
<tr>
<td>21</td>
<td>Redussolution</td>
<td>( 1 ) ( v_{21,ALK} )</td>
<td>( 3.45 ) ( v_{21,ALK} )</td>
<td>( -4.87 ) ( v_{21,ALK} )</td>
<td>( -4.87 ) ( v_{21,ALK} )</td>
<td>( -4.87 ) ( v_{21,ALK} )</td>
</tr>
</tbody>
</table>

Table 2.19: Stoichiometric coefficients of the processes describing simultaneous precipitation and redissolution of phosphorus. The values in this table are based on the assumption that the metal \( Me \) is Ferro (Fe).

### 2.5.3 Limitations of ASM2d

The assumptions and restrictions of the Activated Sludge Model No. 2d are equivalent to the ones of ASM2. So the model is only valid for municipal wastewater. Processes with an overflow of acetate \( (S_A) \) in the aeration tanks of a WWTP cannot be modelled. Furthermore, it is assumed there is sufficient magnesium and potassium in the wastewater. Also in ASM2d the pH should be near neutral and the temperature must be in the range of 10 to 25 degree Celsius.

ASM2d should be used as a basis for the modelling of simultaneous biological phosphorus uptake, nitrification and denitrification. Compared with ASM2 this model will give more accurate results for modelling nitrate and phosphate dynamics.

### 2.6 Activated Sludge Model No. 3

When the Activated Sludge Model No. 1 was introduced in 1987 it became a widely used reference for modelling activated sludge systems. However, there are some defects in the model. In order to repair some of these errors, Activated Sludge Model No. 3 was...
introduced in 1999 by the IAWQ task group [6]. Below is a list of some of the defects of ASM1, which are corrected in ASM3.

- ASM1 does not include kinetic expressions dealing with nitrogen and alkalinity limitations of heterotrophic organisms.
- In ASM1 the components biodegradable soluble and particulate organic nitrogen are used. These are quite hard to measure in the WWTP.
- Kinetics of ammonification cannot be quantified. This means that ASM1 does not contain the exact equations for the ammonification process.
- ASM 1 divides inert particulate organic material depending on its origin. This is not possible in reality.
- The assignment of values to the parameters of the model is difficult. Also the determination of kinetic parameters can be hard.
- ASM1 does not contain the processes for storage of PHA (poly-hydroxy-alkanoates, see ASM2) under aerobic and anoxic conditions.

ASM3 models oxygen consumption, sludge production, nitrification and denitrification for wastewater treatment plants.

### 2.6.1 Components in ASM3

Again, we first look at the components in the model. All components can be found in table 2.20. One important difference, compared with ASM1 and ASM2, is that in ASM3 the soluble and particulate material can be better differentiated with 0.45 micrometer filters. The soluble elements may carry ionic charges, whereas the particulate elements are neutral in the model. New in ASM3 is the component for internal storage products.

<table>
<thead>
<tr>
<th>Notation</th>
<th>Component</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S_O$</td>
<td>Dissolved oxygen, $O_2$</td>
<td>$M(O_2)L^{-3}$</td>
</tr>
<tr>
<td>$S_I$</td>
<td>Inert soluble organic material</td>
<td>$M(COD)L^{-3}$</td>
</tr>
<tr>
<td>$S_S$</td>
<td>Readily biodegradable organic substrates</td>
<td>$M(COD)L^{-3}$</td>
</tr>
<tr>
<td>$S_{NH}$</td>
<td>Ammonium and ammonia nitrogen</td>
<td>$M(N)L^{-3}$</td>
</tr>
<tr>
<td>$S_{N_2}$</td>
<td>Dinitrogen, $N_2$</td>
<td>$M(N)L^{-3}$</td>
</tr>
<tr>
<td>$S_{NO}$</td>
<td>Nitrate and nitrite nitrogen</td>
<td>$M(N)L^{-3}$</td>
</tr>
<tr>
<td>$S_{ALK}$</td>
<td>Alkalinity of wastewater</td>
<td>mol(HCO$^{-}_3$) $L^{-3}$</td>
</tr>
<tr>
<td>$X_I$</td>
<td>Inert particulate organic material</td>
<td>$M(COD)L^{-3}$</td>
</tr>
<tr>
<td>$X_S$</td>
<td>Slowly biodegradable substrates</td>
<td>$M(COD)L^{-3}$</td>
</tr>
<tr>
<td>$X_H$</td>
<td>Heterotrophic organisms</td>
<td>$M(COD)L^{-3}$</td>
</tr>
<tr>
<td>$X_{STO}$</td>
<td>Cell internal storage product of heterotrophic organisms</td>
<td>$M(COD)L^{-3}$</td>
</tr>
<tr>
<td>$X_A$</td>
<td>Nitrifying organisms</td>
<td>$M(COD)L^{-3}$</td>
</tr>
<tr>
<td>$X_{TS}$</td>
<td>Total suspendid solids</td>
<td>$M(TSS)L^{-3}$</td>
</tr>
</tbody>
</table>

Table 2.20: Components of the Activated Sludge Model 3.
2.6.2 Processes in ASM3

In ASM3 only microbiological transformation processes are included. Chemical processes do not appear in the model. In ASM2 there is a chemical process in the phosphorus removal. The processes with their stoichiometry and rate equations can be found in the tables 2.21, 2.22 and 2.23. The hydrolysis process is a bit different compared with ASM1, it is less dominating. AMS3 contains processes for aerobic and anoxic storage of readily biodegradable substrate, which was not available in ASM1.

<table>
<thead>
<tr>
<th>Component → j</th>
<th>Process ↓</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
<th>11</th>
<th>12</th>
<th>13</th>
</tr>
</thead>
<tbody>
<tr>
<td>S O</td>
<td>S I</td>
<td>S S</td>
<td>S S N H</td>
<td>S N O</td>
<td>S HCO</td>
<td>X I</td>
<td>X S</td>
<td>X H</td>
<td>X S TO</td>
<td>X A</td>
<td>X S T O</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1. Hydrolysis</td>
<td>f S I</td>
<td>x 1</td>
<td>y 2</td>
<td>z 1</td>
<td>-1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>-1</td>
</tr>
<tr>
<td>Heterotrophic organisms</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2. Aerobic storage COD</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
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<td></td>
<td></td>
<td></td>
<td>t 2</td>
</tr>
<tr>
<td>3. Anoxic storage COD</td>
<td></td>
<td></td>
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<td></td>
<td></td>
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<td></td>
<td></td>
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<td></td>
<td></td>
<td></td>
<td>t 3</td>
</tr>
<tr>
<td>4. Aerobic growth</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
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<td></td>
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<td></td>
<td>t 4</td>
</tr>
<tr>
<td>5. Anoxic growth</td>
<td></td>
<td></td>
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<td></td>
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<td></td>
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<td></td>
<td>t 5</td>
</tr>
<tr>
<td>6. Aerobic respiration</td>
<td></td>
<td></td>
<td></td>
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<td></td>
<td></td>
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<td></td>
<td></td>
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<td></td>
<td></td>
<td>t 6</td>
</tr>
<tr>
<td>7. Anoxic respiration</td>
<td></td>
<td></td>
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<td></td>
<td></td>
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<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>t 7</td>
</tr>
<tr>
<td>8. Aerobic respiration X S TO</td>
<td></td>
<td></td>
<td></td>
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<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>t 8</td>
</tr>
<tr>
<td>9. Anoxic respiration X S TO</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>t 9</td>
</tr>
<tr>
<td>Autotrophic organisms</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
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<td></td>
<td>t 10</td>
</tr>
<tr>
<td>10. Nitrification</td>
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<td></td>
<td></td>
<td></td>
<td></td>
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<td></td>
<td></td>
<td>t 11</td>
</tr>
<tr>
<td>11. Aerobic respiration</td>
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<td></td>
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<td></td>
<td></td>
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<td></td>
<td></td>
<td></td>
<td>t 12</td>
</tr>
<tr>
<td>12. Anoxic respiration</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
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<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>t 13</td>
</tr>
</tbody>
</table>

Table 2.21: Stoichiometric matrix $\omega_{j,i}$. More information can be found in [6].
### Table 2.22: Composition matrix $l_{k,i}$. Here COD, Nitrogen and the Ionic charge are the conservatives and TSS is the observable. The matrix is used together with the stoichiometric matrix of ASM3 in table 2.21.

<table>
<thead>
<tr>
<th>Process</th>
<th>Rate equation $\rho_j$, all $\rho_j \geq 0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Hydrolysis</td>
<td>$K_X \cdot \frac{X_{A,NO}}{K_{A,NO} + S_{NH}} \cdot X_H$</td>
</tr>
<tr>
<td>Heterotrophic organisms, denitrification</td>
<td>$k_{STO} \cdot \frac{S_O}{K_{O+SO}} \cdot \frac{S_S}{K_S+SS} \cdot X_H$</td>
</tr>
<tr>
<td>2. Aerobic storage COD</td>
<td>$k_{STO} \cdot \frac{S_NO}{K_{NO+SNO}} \cdot \frac{S_S}{K_S+SS} \cdot X_H$</td>
</tr>
<tr>
<td>3. Anoxic storage COD</td>
<td>$\mu_H \cdot \frac{S_O}{K_{O+SO}} \cdot \frac{S_NH}{K_{NH+SNH}} \cdot \frac{S_{HCO}}{K_{HCO+S_{HCO}}} \cdot \frac{S_{STO}}{X_{STO/XH}} \cdot X_H$</td>
</tr>
<tr>
<td>4. Aerobic growth</td>
<td>$\mu_H \cdot \frac{S_NH}{K_{NH+SNH}} \cdot \frac{S_{HCO}}{K_{HCO+S_{HCO}}} \cdot \frac{X_{STO/XH}}{X_{STO/XH}} \cdot X_H$</td>
</tr>
<tr>
<td>5. Anoxic growth</td>
<td>$b_{H,O_2} \cdot \frac{S_O}{K_{O+SO}} \cdot X_H$</td>
</tr>
<tr>
<td>6. Aerobic respiration</td>
<td>$b_{H,NO} \cdot \frac{S_O}{K_{O+SO}} \cdot \frac{S_{NO}}{K_{NO+S_{NO}}} \cdot X_H$</td>
</tr>
<tr>
<td>7. Anoxic respiration</td>
<td>$b_{STO,O_2} \cdot \frac{S_O}{K_{O+SO}} \cdot X_{STO}$ with $b_{STO,O_2} \geq b_{H,O_2}$</td>
</tr>
<tr>
<td>8. Aerobic respiration of $X_{STO}$</td>
<td>$b_{STO,NO} \cdot \frac{K_A}{K_{O+SO}} \cdot \frac{S_{NO}}{K_{NO+S_{NO}}} \cdot X_{STO}$ with $b_{STO,NO} \geq b_{H,NO}$</td>
</tr>
<tr>
<td>9. Anoxic respiration of $X_{STO}$</td>
<td>$\mu_A \cdot \frac{S_O}{K_{A,O+SO}} \cdot \frac{S_{NH}}{K_{A,NH+S_{NH}}} \cdot \frac{S_{HCO}}{K_{A,HCO+S_{HCO}}} \cdot X_A$</td>
</tr>
<tr>
<td>Autotrophic organisms, nitrification</td>
<td>$b_{AO_2} \cdot \frac{S_O}{K_{O+SO}} \cdot X_A$</td>
</tr>
<tr>
<td>10. Nitrification</td>
<td>$b_{A,NO} \cdot \frac{K_A}{K_{O+SO}} \cdot \frac{S_{NO}}{K_{NO+S_{NO}}} \cdot X_A$</td>
</tr>
<tr>
<td>11. Aerobic respiration</td>
<td></td>
</tr>
<tr>
<td>12. Anoxic respiration</td>
<td></td>
</tr>
</tbody>
</table>

Table 2.23: Rate equations of Activated Sludge model No. 3. A detailed discription and example values of the parameters can be found in the article by Gujer et al [6].

Other processes in AMS3 are the aerobic and anoxic growth of heterotrophs. Another big difference with ASM1 are the aerobic and anoxic endogenous respiration. These processes describe all forms of biomass loss and energy requirements not associated with growth. In ASM1 the decay process was linked with the growth process. One remark is that anoxic endogenous respiration is generally slower than aerobic endogenous respiration. The last two processes in ASM3 are the aerobic and anoxic respiration of storage products.
which are analogous to endogenous respiration.

ASM3 contains a more detailed description of cell internal processes, like the storage of material. It also performs better if we look at the adjustment of decay processes under different environmental conditions.

As said before ASM3 is given in three tables. In the first tables, 2.21 and 2.22, the stoichiometric components \((\nu_{ij})\) are given together with the composition matrix. The latter is not widely known. The stoichiometric matrix contains continuity equations (summing over the row of the matrix), as seen with ASM1. To give all elements from the stoichiometric matrix the same units in the continuity equation, the composition matrix is introduced. This leads to the following formula for continuity equations:

\[
\sum_i \nu_{i,j} l_{i,k} = 0 \text{, for } i = 1, ..., 12.
\]

(2.10)

One additional equation is introduced for the stoichiometric coefficients of the observable \(X_{TS}\). This equation is given as

\[
\nu_{j,13} = \sum_i \nu_{j,i} l_{4,i} \text{, for } i = 8, ..., 12.
\]

(2.11)

In the third table of the model 2.23 the process rate equations can be found. Just like the previous activated sludge models, the kinetics are based on a combination of simple switching functions together with additional rate constants. One of these constants are the kinetic parameters \(k\). These parameters depend on the temperature of the wastewater. For different temperatures it is recommended to interpolate the parameter with the following equation:

\[
k(T) = k(20) \exp(\Theta_T \cdot (T - 20))
\]

(2.12)

with \(T\) the temperature in degrees Celsius and

\[
\Theta_T = \frac{\ln(k(T_1)/k(T_2))}{T_1 - T_2},
\]

(2.13)

where \(k(T_i)\) is a known value of the parameter at temperature \(T_i\) with \(i = 1, 2\).

One small remark: the temperature dependence of kinetic parameters is for the first time introduced in the article of Activated Sludge model No.3. In the previous models this temperature dependence is not mentioned.

### 2.6.3 Limitations of ASM3

The complexity of the Activated Sludge Model No.3 is comparable to the complexity of ASM1. The model is unfortunately not tested with a large variety of experimental data. Therefore it remains to be seen if all limitations of ASM1 have successfully been eliminated. ASM3 also has some limitations. The model is only valid for a temperature from 8
to 23 degree Celsius. Also the pH of the wastewater must be near neutral in the range of 6.5 to 7.5.

ASM3 does not contain any process describing the behaviour of biomass in an anaerobic environment, just as ASM1. Simulation of systems with large fractions of anaerobic reactor volumes may lead to large errors in the solution of the model. Also ASM3 does not tells us something about nitrite inhibition. Just as AMS1, ASM3 can only be used for municipal wastewater, high concentrations of organic material in the wastewater can be limiting the results of the model.

2.7 A Comparison of the Activated Sludge Models

In the sections above all four Activated Sludge Models are introduced. In this section a small comparison between the models is made. First we look at the Activated Sludge Model No. 1 and No. 3. For both models a schematic representation can be found in figure 2.1.

![Figure 2.1: Schematic representation of the components and processes in ASM1 and ASM3. The figure can be found in [6].](image)

One big difference between the models is that the nitrifiers (or autotrophs) and heterotrophs are strictly separated in ASM3. In ASM1 these are connected by the nitrifiers, which contribute to heterotrophic growth. Also only two oxygen entry points are in the model. In AMS3 there are in total 5 points in the processes where dissolved oxygen is entered in the model. Also ASM3 contains information about the cell internal storage of materials. In ASM1 this is not treated.

Due to the differences described above the models are quit different from each other. Not all components are the same. In ASM3 there are components representing the internal storage. Also the rate equations between both models are quite different. The basis of these equations are constant parameters (conversion rates or kinetic parameters) and switching
functions. For some processes in ASM3 there are more switching functions used, compared with ASM1, because a few processes in ASM3 depend on more components of the model compared with ASM1.

The biggest difference between ASM1, ASM3 and both Activated Sludge Models No. 2 and No. 2d is that the latter contain the processes for phosphorus removal. Therefore the number of components in the model is increased to 20 in ASM2. Also the number of processes is increased from 8 to 19 in ASM2, compared with ASM1. Model No. 2d even has two additional processes, which makes a total of 21. Both, ASM2 and ASM2d, are more complex to use in practice because the are much larger compared with ASM1. They give however a better representation for wastewater treatment plants. ASM2 and ASM2d are slightly different, because in ASM2d it is assumed that the organisms removing the phosphate also can denitrify.

ASM2 and ASM2d are, just like the other models, introduced in matrix notation with stoichiometric parameters and rate equations. Although the models are quite different, the basis of the models is the same. So the rate equations consists of (constant) parameters and switching functions. ASM2 and ASM2d are more complex due to the fact that the model contains more components and processes. There are also more relations between the processes in the model, resulting in rate equations with more terms.

All four models use continuous switching functions in the rate equations. These continuous functions have the general forms

\[
\frac{S_x}{S_x + K_x} \quad (2.14)
\]

and

\[
\frac{K_x}{S_x + K_x} \quad (2.15)
\]

Here \(S_x\) is a soluble component of the model, where \(x\) specifies the exact element. For example \(S_x\) is equal to the dissolved oxygen \(S_{O_2}\). Parameter \(K_x\) is kinetic parameter depending on the component of the model. In most cases it is the concentration of the component \(x\) for which the half-maximum specific growth rate is achieved in the wastewater.

As said before, switching functions are introduced to ‘turn on and off’ processes in the Activated Sludge Models. If in switching function \(2.14\) the concentration of \(S_x\) approaches zero the corresponding process is turned off, because the value of the function becomes zero. If, however \(S_x\) approaches zero, but equation \(2.15\) is used, the process is turned on, because the value of the switching function approaches 1. Together with the stoichiometric parameters we can model growth (and other processes in wastewater treatment) under different environmental conditions using these switching functions.
Chapter 3

Modelling of Flow

Until now only the biological processes in a wastewater treatment plant are discussed, which can be modelled with the Activated Sludge Models. In these models only reaction terms are given. In a tank (or reactor) all material in the wastewater is distributed in some way. This mixing is a 3-dimensional process, which could be solved with Computational Fluid Dynamics. There are also other, more simple methods describing this process. This chapter introduces the modelling of fluid flow.

3.1 Tanks-in-series

The tanks-in-series model is an empirical model, meaning that it depends on certain measurements in the wastewater treatment plant. The model consists of small tanks where the wastewater is assumed to be homogeneous distributed. In each tank one of the Activated Sludge Models is used to model all biological removal processes of a wastewater treatment plant. These small tanks are connected to each other in series (hence the name tanks-in-series). By increasing the number of tanks in the model it is possible to model a large tank with all biological processes. The biggest challenge using the tanks-in-series model is the determination of the number of tanks which should be used. Also the corresponding in- and outflow for each small tank needs to be determined. The combination of tanks with (different) in- and outflow for each tank makes it possible to model the total flow in a wastewater treatment plant. Together with a Activated Sludge Model also the biological processes are modelled.

If the activated sludge reactor with aeration of a wastewater treatment plant has the shape of a rectangle the number of tanks can be determined using the equation

\[ i = \frac{7.4}{B \cdot H} \cdot L \cdot Q_{in} \cdot (1 + R). \]

(3.1)

This equation (found in [18]) is only valid for values of the variables in a certain range, see table 3.1.
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<table>
<thead>
<tr>
<th>Notation</th>
<th>Variable and unit</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>L</td>
<td>Length of the reactor ((m))</td>
<td>28 – 500</td>
</tr>
<tr>
<td>B</td>
<td>Width of the reactor ((m))</td>
<td>2 – 20</td>
</tr>
<tr>
<td>H</td>
<td>Height of the reactor ((m))</td>
<td>2.4 – 6.0</td>
</tr>
<tr>
<td>R</td>
<td>Rate of circulation ((-))</td>
<td>0.7 – 1.5</td>
</tr>
<tr>
<td>(\Theta) = (\frac{V_{tot}}{Q_{m}(1+R)})</td>
<td>(\Theta) time in the reactor ((\text{h}))</td>
<td>1.3 – 3.0</td>
</tr>
<tr>
<td>(V_{tot})</td>
<td>total volume of reactor ((m^3))</td>
<td></td>
</tr>
</tbody>
</table>

Table 3.1: Variables of equation 3.1 used for determining the number of tanks in the tanks-in-series model.

There are also other ways for determining the number of tanks in the model. For example, a tracer study could be used. This method requires a collection of experimental data from the wastewater treatment plant. A fixed amount of tracer is added to the wastewater. The concentration of the tracer can be coupled to the tanks in series model. A short introduction is given here, see also [18].

\[
\begin{align*}
Q & \rightarrow n_1 \rightarrow C_1Q \rightarrow n_2 \rightarrow C_2Q \rightarrow \ldots \rightarrow C_{i-1}Q \rightarrow n_i \rightarrow C_iQ \\
\end{align*}
\]

Figure 3.1: The tanks-in-series model. Each tank has a volume \(V/i\), giving a total volume of \(V\). The volumetric throughput is given by \(Q\) and \(n\) the total amount of tracer added to the wastewater treatment plant. \(n_m\) is the amount of tracer in each tank.

Suppose there are \(i\) identical reactors (figure 3.1) with a total volume \(V\), so each reactor has a volume \(Vi^{-1}\). Let \(Q\) be the volumetric throughput. An amount of \(n\) mol tracer is added to the wastewater, which is assumed not to contain any tracer material until that moment. The concentration of tracer in tank \(m\) \((m \leq i)\) is given by \(C_m = n_m/(Vi^{-1}) = n_m/iV^{-1}\). The amount of tracer transported between the tanks is given by \(QC_m\). A mass-balance (input-output-reaction = accumulation) over the first tank for the amount of tracer can be given:

\[
0 - \frac{n_1Q}{V} - 0 = \frac{dn_1}{dt}.
\]

Integration (with proper initial condition, \(n_1 = n\) at \(t = 0\)) gives \(n_1 = ne^{-\frac{Qt}{V}}\). In the same way a mass-balance for \(n_m\) for the second tank can be given:

\[
\frac{n_1iQ}{V} - \frac{n_2iQ}{V} - 0 = \frac{dn_m}{dt}.
\]
3.2. COMPUTATIONAL FLUID DYNAMICS

Substitution of \( n_1 \) and integration gives the solution

\[
n_2 = n \frac{Q_i t}{V} e^{-\frac{Q_i t}{V}}.
\]

In general it can be concluded that for tank \( m \) the amount of tracer can be given by

\[
n_m = \frac{n}{(m - 1)!} \left( \frac{Q_i t}{V} \right)^{m-1} e^{-\frac{Q_i t}{V}}.
\]

Using this last equation the amount of tracer \( n_m \) in tank \( m \) can be calculated and using \( n_m \) the concentration tracer \( C_m \) can be calculated. This also holds for the last tank, with number \( m = i \), making it possible to calculate the concentration of tracer in the last tank \( i \). Taking \( C_0 = nV^{-1} \) a plot of the curve \( C_i/C_0 \) versus time can be made. This curve can fit the measured tracer concentration in a wastewater treatment plant. By taking different numbers of \( i \) a curve can be chosen which gives the best approximation of the experimental data. The corresponding \( i \) is the number of tanks which is needed in the tanks-in-series model. More detailed information about the tanks in series can be found in chapter 14 of Chemical Reaction Engineering by Octave Levenspiel [12]. Two examples of computer packages that use the tanks-in-series model for a wastewater treatment plant are SIMBA and WEST2009. In both packages it is possible to choose between the different Activated Sludge Models. More information about SIMBA can be found in the SIMBA-protocol [1].

3.2 Computational Fluid Dynamics

The tanks-in-series is a very simple model for the flow and mixing in the tanks of a wastewater treatment plant. It is also possible to use Computational Fluid Dynamics (CFD) for the modelling of fluid flow and mixing of elements in a reactor. This will give accurate results, but the calculations can take a lot of time. In the next sections of this chapter the equations for the modelling of flow with Computational Fluid Dynamics will be treated. We will also take a look at the transport of the components in the wastewater.

3.2.1 The Navier-Stokes Equations

Fluid flow can be described with the Navier-Stokes equations. A complete derivation of these equations can be found in the lecture notes of Veldman [21]. In this section the equations will be discussed. The basis of Navier-Stokes equations are conservation of mass and conservation of momentum.

First we take a look at the conservation of mass, which is given by the equation

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) + \frac{\partial}{\partial y}(\rho v) + \frac{\partial}{\partial z}(\rho w) = 0,
\]

(3.3)
or in vector notation as
\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0. \tag{3.4}
\]
Here \( \mathbf{u} = (u, v, w) \) is the velocity vector and \( \rho \) is the density. The equation is also called the continuity equation. It can be written as
\[
\frac{D \rho}{D t} + \rho \nabla \cdot \mathbf{u} = 0, \tag{3.5}
\]
where \( \frac{D \rho}{D t} \) is the Lagrangian derivative: \( \frac{\partial \rho}{\partial t} + \mathbf{u} \cdot \nabla \rho \). If, a fluid is incompressible, hence the density (\( \rho \)) is constant, the continuity equation reduces to
\[
\nabla \cdot \mathbf{u} = 0. \tag{3.6}
\]

Next, we consider the momentum equation, which is in vector notation given as
\[
\rho \frac{D \mathbf{u}}{D t} = -\nabla p + \rho \mathbf{F}. \tag{3.7}
\]
In this equation, sometimes called the Euler momentum equation, \( p \) is the pressure and \( \mathbf{F} \) are additional forces acting on the fluid.

In [19] a more general notation for above equations is given. Also a third equation describing the conservation of energy is added. If, however, an incompressible flow (density \( \rho \) is constant) is treated, than the energy equation can be replaced with the condition of incompressibility. What remains is equation \( \text{(3.5)} \) and the equation of conservation of momentum. In this last equation a term for viscous stresses is added. The complete Navier-Stokes equations for incompressible flow of an fluid are given as
\[
\nabla \cdot \mathbf{u} = 0, \tag{3.8}
\]
\[
\frac{D \mathbf{u}}{D t} = -\frac{1}{\rho} \nabla p + \nu \Delta \mathbf{u}. \tag{3.9}
\]
In equation \( \text{(3.9)} \) \( \nu = \frac{\eta}{\rho} \) is the kinematic viscosity, where \( \eta \) is the dynamic viscosity.

The Navier-Stokes equations cannot be solved analytically in most cases. Therefore numerical methods are needed. This subject is treated by Veldman in Computational Fluid Dynamics (see also [19]).

When treating the fluid flow one important dimensionless number appears in the theory. This is the Reynolds number which is a measure for the ratio between inertia forces and viscous forces. It is named after Osborne Reynolds and given as
\[
Re = \frac{\rho U L}{\eta} = \frac{UL}{\nu}, \tag{3.10}
\]
with \( U \) the characteristic velocity and \( L \) the characteristic length. When the Reynolds number is large (\( Re >> 1 \)) the influence of the viscosity of the fluid has very little influence on the fluid flow. Only in the direct surroundings of an obstacle effects can be visible. In general a boundary layer is present, where the flow becomes turbulent. In the next section the modelling of turbulent flow will be treated.
3.2. COMPUTATIONAL FLUID DYNAMICS

3.2.2 Modelling of Turbulent Flow

In a reactor of a wastewater treatment plant the fluid flow can become turbulent. The incompressible Navier-Stokes equations describe this complete turbulent flow. Unfortunately, it is not yet possible to solve these equations numerically for a turbulent flow. The computational power of computers is too small. For the calculation of a turbulent flow a model exists, which can be numerically solved on a regular personal computer. This turbulence model is called the $k - \varepsilon$ model (see [3,17]), which is also used in the computer program COMSOL.

The basis of a turbulence model are the so-called Reynolds-average equations [20]. It is assumed that the variables in the Navier-Stokes equations can be divided into a mean value and a fluctuation. For example,

$$u = \overline{u} + u',$$

with $\overline{u}$ the mean value over a time interval $T$:

$$\overline{u}(x, t) = \frac{1}{T} \int_t^{t+T} u(x, \tau)d\tau. \quad (3.11)$$

Further the approximation

$$\int_t^{t+T} u' d\tau = 0$$

holds by the assumption that the mean value is a constant over the interval $T$. The pressure is also divided into a mean value and fluctuation, $p = \overline{p} + p'$. Using the vector notation, the Navier-Stokes equations are in this case

$$\nabla \cdot \overline{u} = 0, \quad (3.12)$$

$$\rho \frac{\partial \overline{u}}{\partial t} + \rho \overline{u} \cdot \nabla \overline{u} + \nabla \cdot (\rho u' \times u') = -\nabla p + \nabla \cdot \eta \left( \nabla \overline{u} + (\nabla \overline{u})^T \right) + F, \quad (3.13)$$

where $\times$ is the outer vector product. The term $\overline{(\rho u' \times u')}$ is called the Reynolds stress tensor. The equations 3.13 and 3.13 are the Reynolds-averaged Navier-Stokes equations (RaNS).

Solving these new equations gives some problems. For the new unknowns $u'$, no equation is available, which solves the set of equations. Therefore some additional equations have to be found. This is called the closure problem. A common way to model turbulence is to assume that the turbulence is of diffusive nature. With this assumption the Reynolds stress term can be expressed by:

$$\rho \left( u' \times \overline{u} \right) = \frac{2}{3} \rho k - \eta_T \left( \nabla \overline{u} + (\nabla \overline{u})^T \right). \quad (3.14)$$

Here $\eta_T$ is the eddy viscosity (also known as turbulent viscosity) and $k$ the turbulent kinetic energy.
The $k-\varepsilon$ model for turbulence was introduced in 1972. In the model, first the turbulent kinetic energy is introduced in terms of $u'$ [2],

$$k = \frac{1}{2}(\rho u' \times u').$$

A transport equation is set up for $k$, which consists of convection, diffusion and production. Turbulent viscosity is modelled by

$$\eta_T = \rho c_\mu \frac{k^2}{\varepsilon},$$

(3.15)

where $\varepsilon$ is the dissipation (the loss of energy) of the kinetic energy. The transport equation is given by

$$\rho \frac{\partial k}{\partial t} - \nabla \cdot \left[ \left( \eta + \frac{\eta_T}{\sigma_k} \right) \nabla k \right] + \rho \mathbf{u} \cdot \nabla k = \frac{1}{2} \eta_T \left( \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right)^2 - \rho \varepsilon.$$  

(3.16)

Also an equation has to be found for $\varepsilon$, which is unfortunately not possible from physical insight. The equation most used in practice and also used in COMSOL Multiphysics is given by

$$\rho \frac{\partial \varepsilon}{\partial t} - \nabla \cdot \left[ \left( \eta + \frac{\eta_T}{\sigma_\varepsilon} \right) \nabla \varepsilon \right] + \rho \mathbf{u} \cdot \nabla \varepsilon = \left[ \frac{1}{2} c_{\varepsilon 1} \eta_T \left( \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right)^2 - \rho c_{\varepsilon 2} \varepsilon \right] \frac{\varepsilon}{k},$$

(3.17)

which has more or less the same structure as the equation for the turbulent kinetic energy. The constants in the equation above are determined from experimental data and are usually chosen as in table 3.2.

<table>
<thead>
<tr>
<th>Constant</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_\mu$</td>
<td>0.09</td>
</tr>
<tr>
<td>$c_{\varepsilon 1}$</td>
<td>1.44</td>
</tr>
<tr>
<td>$c_{\varepsilon 2}$</td>
<td>1.92</td>
</tr>
<tr>
<td>$\sigma_k$</td>
<td>1.00</td>
</tr>
<tr>
<td>$\sigma_\varepsilon$</td>
<td>1.30</td>
</tr>
</tbody>
</table>

Table 3.2: Constants in the $k-\varepsilon$ model.

The equations of the $k-\varepsilon$ turbulence model are two additional equations. The model is therefore a two-equation model. This also means that the continuity and momentum equation, of the Reynolds-averaged Navier-Stokes equations still hold. All four equations together model a turbulent flow.

There are also other models describing turbulent flow. These models are not used very often in the calculations of turbulent flows. An example is the $k-\omega$ turbulence model. This model is just like the $k-\varepsilon$ model a two equation model, describing the turbulence kinetic energy $k$ and a specific dissipation $\omega$. The model is used in the same way as the $k-\varepsilon$ model.
3.2. Modelling of Mass Transport

In the previous sections the modelling of fluid flow is introduced. The Activated Sludge Model only gives the reaction terms for the components in the wastewater entering a wastewater treatment plant. Until now the transport of the components in the wastewater is not modelled.

For the transport of a solute two transport mechanisms can be distinguished, namely convection and diffusion \[19\]. Convection is the transport due to the motion of the medium, in this case water. Diffusion is the transport caused by a difference in concentration. In general, we can say that the material is transported from a high concentration to an area with a low concentration. Let \( c(x, t) \) be the concentration, depending on space \( x = (x, y, z) \) and time \( t \). Again it is assumed that the flow is incompressible (density \( \rho \) is constant), with a velocity \( u(x,t) \).

The equation for the concentration depends on space and time and can be derived from a conservation law. Consider an arbitrary volume \( \Omega \) with boundary \( \Gamma \) and normal \( n \) pointing outward, see figure 3.2.

\[ \text{Figure 3.2: Arbitrary volume used for the derivation of the mass transport equation.} \]

Now assume that the amount of solute in the volume is decreased due to outward transport through the boundary. The transport by convection is given by

\[ \int_{\Gamma} cu \cdot n \, d\Gamma, \]

and the diffusive transport is

\[ \int_{\Gamma} -k \nabla c \cdot n \, d\Gamma. \]

The diffusion is proportional to the gradient of the concentration, with diffusion coefficient \( k \geq 0 \). The conservation of mass in the volume becomes

\[ \int_{\Omega} \frac{\partial c}{\partial t} \, d\Omega = - \int_{\Gamma} (cu - k \nabla c \cdot n) \, d\Gamma, \]
Where the integral over the volume represents accumulation. Applying Gauss’s Theorem this can be rewritten into

\[ \int_{\Omega} \frac{\partial c}{\partial t} d\Omega = - \int_{\Omega} \nabla \cdot (c u - k \nabla c \cdot n) d\Omega. \]

Since this holds for any arbitrary volume \( \Omega \), it follows that

\[ \frac{\partial c}{\partial t} + \nabla \cdot (c u - k \nabla c) = 0. \] (3.18)

The equation above is called the convection-diffusion equation. It is written in a so-called divergence form. If the medium is incompressible, so \( \nabla \cdot u = 0 \), the equation can be written as

\[ \frac{\partial c}{\partial t} + u \cdot \nabla c - \nabla \cdot (k \nabla c) = 0. \]

Finally, a reaction term \( R \) can be added to the equation, which can model a certain production or consumption of solute in the medium. The convection-diffusion equation becomes

\[ \frac{\partial c}{\partial t} + u \cdot \nabla c - \nabla \cdot (k \nabla c) = R. \] (3.19)

Using equation 3.19 the transport of component in the wastewater of a treatment plant can be modelled. When the fluid flow becomes turbulent, this also influences the mixing of the components in the tank. This so-called turbulent mixing is still modelled with the convection-diffusion equation, with a modified diffusion coefficient \[2\]. This diffusion-coefficient is given by

\[ k = \frac{\eta_T \rho}{\rho}, \] (3.20)

with \( \eta_T \) the turbulent viscosity and \( \rho \) the liquid density.

### 3.2.4 Modelling of Mass Transfer

In some tanks of a wastewater treatment plant an aeration process is used. In most cases air is added to the wastewater from the bottom of a tank. This air contains oxygen, which is used by the bacteria performing the biological processes. The oxygen, nitrogen and carbon dioxide dissolve in the wastewater. This process is a typical mass transfer process. In this section a model for mass transfer between a gas and liquid is given.

Mass transfer depends on the interfacial area between two phases \[2\]. First we expect that the amount of mass transferred is proportional to the concentration difference and the interfacial area \[4\]:

\[ \text{(rate of mass transferred)} = k \left( \frac{\text{interfacial area}}{\text{concentration difference}} \right), \] (3.21)
where $k$ is the mass transfer coefficient. Dividing both sides of this equation by the area we get

$$N = k(c^* - c), \quad (3.22)$$

with $N$ flux at the interface, $c^*$ the concentration at the interface and $c$ the concentration in the liquid. The flux contains in this case both convection and diffusion. Mass transfer coefficient $k$ is a rate constant determining the speed of mass transfer.

Before calculating the mass transfer, first the interfacial area needs to be determined. When gas dissolves into a liquid, the number of gas bubbles is needed for this determination. Assume that gas bubbles can expand and shrink, but cannot completely vanish, merge or split. Then the conservation of the number density $n$ (with unit $1/m^3$) of the gas bubbles gives

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{v}) = 0, \quad (3.23)$$

where $\mathbf{v}$ is the velocity of the gas. Solving above equation for $n$ gives, together with the fraction of gas $\phi_g$, the interfacial area per volume ($m^2/m^3$):

$$a = (4n\pi)^{1/3}(3\phi_g)^{2/3}. \quad (3.24)$$

COMSOL Multiphysics uses a model for mass transfer following the two-film theory. Let $N$ (unit: mol/(sm$^2$)) be the molar flux per interfacial area. The mass transfer between a gas and liquid is given by

$$m_{gl} = NMa. \quad (3.25)$$

Here $M$ is the molar mass of the gas, $a$ the interfacial area and $N$ is determined by

$$N = k(c^* - c),$$

where $k$ is the mass transfer coefficient, $c$ the concentration of the gas dissolved in the liquid. The equilibrium concentration $c^*$ of gas in the liquid can be found with Henry’s law:

$$c^* = \frac{p + p_{ref}}{H},$$

where $H$ is Henry’s constant. The concentration of the dissolved gas $c$ can be modelled using the convection-diffusion equation found in section 3.2.3:

$$\frac{\partial c}{\partial t} + \nabla \cdot (cu) - \nabla \cdot (D\nabla c) = Na. \quad (3.26)$$

### 3.2.5 Using the Models

All models described in the previous sections are partial differential equations. Solving these equations in a certain domain require some conditions on the boundary of that domain. For example, using the incompressible Navier-Stokes equations can require a velocity profile on the inlet boundary or a pressure condition on the outlet boundary. Unfortunately, the partial differential equations can not be solved analytically in most cases. Numerically a solution can be found, using for example the finite element method.
Chapter 4

The Finite Element Method

The mathematical models introduced in the previous section are incorporated in COMSOL Multiphysics 3.5a. This program uses the finite element method for solving the equations. First a mesh over the domain has to be made. In general this mesh consists of triangles, the so-called elements.

Once the mesh is made, approximations are introduced to the dependent variables. The idea is that a variable is approximated by a function that can be described with a finite number of parameters, the so-called degrees of freedom. Inserting this approximation in the equation generates a system of equations for the degrees of freedom. This system can be solved for the degrees of freedom, resulting in a solution for the unknown variable.

4.1 General Idea

In this simple example the idea of the finite element method is discussed. Only linear elements in one dimension are treated, see the reference guide of COMSOL [2]. Consider an interval \( x \) from 0 to 2 and let the mesh consists of two equal elements. This gives two intervals: \( 0 < x < 1 \) and \( 1 < x < 2 \). Let \( u(x) \) be the variable, which we want to solve using the finite element method. A linear element means that on each mesh interval the continuous function \( u \) is linear. It follows that characterizing \( u \) unique only the values in the node points \( x_1 = 0, x_2 = 1 \) and \( x_3 = 2 \) are needed. Denote these as \( U_1 = u(0), U_2 = u(1) \) and \( U_3 = u(2) \). These are the degrees of freedom.

Now it is possible to write \( u(x) \) in terms of the degrees of freedom:

\[
\begin{align*}
u(x) &= U_1 \phi_1(x) + U_2 \phi_2(x) + U_3 \phi_3(x) \\
&= \sum_{i=1}^{3} U_i \phi_i(x)
\end{align*}
\] (4.1)

where \( \phi_i(x) \) are certain piecewise functions. These functions need to be linear on the mesh interval and should equal 1 in the point \( i \), while it should be zero in the other points. An
example of such a function would be

\[ \phi_1(x) = \begin{cases} 1 - x & \text{if } 0 \leq x \leq 1 \\ 0 & \text{if } 1 \leq x \leq 2 \end{cases} \tag{4.2} \]

The functions \( \phi_i \) are called the basis functions. The set of functions \( u(x) \) is a linear function space which is called the finite element space.

![1 dimensional example for the finite element method. A mesh is made and both a linear and quadratic basis function are used.](image)

To increase the accuracy of the method other basis functions can be used. We can use, for example quadratic elements. This implies that for each mesh interval the function is a second-order polynomial. Consider the same example as above, with two additional nodes \( x_4 = 0.5 \) and \( x_5 = 1.5 \). Now on each mesh interval the second-degree polynomial is determined by the degrees of freedom at the endpoints and the midpoint. In this case we get

\[ u(x) = U_1 \phi_1(x) + U_2 \phi_2(x) + U_3 \phi_3(x) + U_4 \phi_4(x) + U_5 \phi_5(x) \tag{4.3} \]

Again \( \phi_i \) are the basis functions, which should be quadratic, equal to 1 in node point \( i \) and zero in all other node points. An example would be

\[ \phi_1(x) = \begin{cases} (1 - x)(1 - 2x) & \text{if } 0 \leq x \leq 1 \\ 0 & \text{if } 1 \leq x \leq 2 \end{cases} \tag{4.4} \]

Solving the degrees of freedom \( U_i \) will give, together with the linear or quadratic basis functions, a numerical solution for the unknown variable \( u \). An illustration can be found in figure 4.1.

### 4.2 Finite Elements in 2D

The finite element method in two dimensions can be explained using an example problem [10]. The following description can be found in the book by Saad [10]. Consider therefore
4.2. **FINITE ELEMENTS IN 2D**

the Poisson equation on a bounded domain \( \Omega \in \mathbb{R}^2 \) with a Dirichlet condition on boundary \( \Gamma \),

\[
- \left( \frac{\partial^2 u}{\partial x_1^2} + \frac{\partial^2 u}{\partial x_2^2} \right) = f \quad \text{in } \Omega, \quad (4.5)
\]

\[
u = 0 \quad \text{on } \Gamma \quad (4.6)
\]

An essential part of the finite element method is Green’s formula, which is

\[
\int_{\Omega} \nabla v \cdot \nabla u \, dx = - \int_{\Omega} v \Delta u \, dx + \int_{\Gamma} v \nabla u \cdot \mathbf{n} \, ds. \quad (4.7)
\]

Solving the Possion equation \( \text{(4.6)} \) numerically with finite elements it is necessary to take approximations for the unknown function \( u \) and translate the equations into a system. In the previous section two ideas for an approximation of \( u \) are given. For the system of equations it is common to use the weak formulation of the problem. Define

\[
a(u, v) \equiv \int_{\Omega} \nabla u \cdot \nabla v \, dx = \int_{\Omega} \left( \frac{\partial u}{\partial x_1} \frac{\partial v}{\partial x_1} + \frac{\partial u}{\partial x_2} \frac{\partial v}{\partial x_2} \right) \, dx,
\]

\[
(f, v) \equiv \int_{\Omega} f v \, dx.
\]

The functional \( a \) has the property that it is bilinear, meaning that it is linear with respect to \( u \) and \( v \). That is,

\[
a(\mu_1 u_1 + \mu_2 u_2, v) = \mu_1 a(u_1, v) + \mu_2 a(u_2, v) \quad \forall \mu_1, \mu_2 \in \mathbb{R},
\]

\[
a(u, \lambda_1 v_1 + \lambda_2 v_2) = \lambda_1 a(u, v_1) + \lambda_2 a(u, v_2) \quad \forall \lambda_1, \lambda_2 \in \mathbb{R},
\]

Further we see that \( (u, v) \) denotes the \( L_2 \)-inner product of \( u \) and \( v \) in \( \Omega \):

\[
(u, v) = \int_{\Omega} u(x)v(x) \, dx.
\]

For functions, which satisfy the Dirichlet Boundary condition, Green’s formula shows that

\[
a(u, v) = - (\Delta u, v). \quad \text{Now, the weak formulation for the Poisson equation consists of selection a subspace } V \text{ of } L^2 \text{ and defining the following problem:}
\]

\[
\text{Find } u \in V \text{ such that } a(u, v) = (f, v), \quad \forall v \in V, \quad (4.8)
\]

which is called the Galerkin condition. From the definition of the weak form we see that space \( V \) only requires the inner product of the gradients of \( u \) and \( v \) and that the functions \( f \) and \( v \) should be \( L^2 \) integrable. A general choice of \( V \) is \( H^1(\Omega) \), a space of all functions with derivatives of the first order in \( L^2 \). However, this space does not take into account the boundary condition \( u = 0 \). The functions in \( V \) should be zero on the boundary \( \Gamma \). Giving the space \( H^1_0(\Omega) \).
Figure 4.2: Example of a domain covered by a triangular mesh. Figure originally from Saad [10].

In the finite element method the weak formulation is approximated by a finite dimensional problem. This can be done by replacing $V$ by a subspace of functions that are defined as low-degree polynomials on the elements of the original domain. A mesh is made for $\Omega$ which consists of triangles, see figure 4.2. The original domain is now approximated by the union $\Omega_h$ of $m$ triangles $K_i$,

$$\Omega_h = \bigcup_{i=1}^{m} K_i.$$  

For each triangle in the mesh it must hold that no vertex lies on the edge of another triangle. The mesh size $h$ is defined as the maximum of the length of the longest side of all triangles:

$$h = \max_{i=1,...,m} \text{diam}(K_i),$$

with $\text{diam}(K_i)$ the longest side of the triangle. Now define the finite dimensional space $V_h$ consisting of all piecewise linear and continuous functions on the polygonal region $\Omega_h$ and are zero on the boundary of this region $\Gamma_h$. That is

$$V_h = \{ \phi|\phi|_{\Omega_h}\text{continuous, } \phi|_{\Gamma_h} = 0, \phi|_{K_i}\text{linear } \forall i \}.$$  \hspace{1cm} (4.9)

Suppose that $x_j \ (j = 1...n)$ are the nodes of the triangular mesh, then a function $\phi_j$ can be associated with each node (see also the previous section). The family of functions $\phi_j$ must satisfy the following condition:

$$\phi_j(x_i) = \delta_{ij} = \begin{cases} 1 & \text{if } x_i = x_j \\ 0 & \text{if } x_i \neq x_j \end{cases}.$$  

These conditions define $\phi_i \ (i = 1,...,n)$ uniquely. The functions are also a basis of the space $V_h$. Each function of $V_h$ can be expressed as

$$\phi(x) = \sum_{i=1}^{n} U_i \phi_i(x).$$
The approximation in the finite element method consists of writing the Galerkin condition for functions in \( V_h \). The approximated problem is now formulated as:

Find \( u \in V_h \) such that \( a(u, v) = (f, v), \forall v \in V_h. \) (4.10)

Since \( u \) is in \( V_h \) there are \( n \) degrees of freedom and because of the linearity of \( a \) with respect to \( v \) it is only necessary to impose the condition \( a(u, \phi_i) = (f, \phi_i) \) for \( i = 1, ..., n \). This gives \( n \) constraints. Now suppose that the desired solution of \( u \) can be written in terms of the basis \( \phi_i \),

\[
  u = \sum_{i=1}^{n} U_i \phi_i(x).
\]

Substitution in the approximated problem gives the linear problem:

\[
  \sum_{j=1}^{n} \alpha_{ij} U_i = \beta_i, \quad (4.11)
\]

with \( \alpha_{ij} = a(\phi_i, \phi_j) \) and \( \beta_i = (f, \phi_i) \) for \( i = 1, ..., n \). These equations form a linear system \( Ax = b \), in which the elements of \( A \) are \( \alpha_{ij} \). \( x \) is the vector of unknowns \( U_i \) and \( b \) contains the \( \beta_i \). This system of equations can be solved using standard numerical mathematics.

It turns out that \( A \) is a symmetric positive definite matrix and is also sparse. In practice, the matrix \( A \) can be build by summing up all the contributions of all triangles using the formula

\[
  a(\phi_i, \phi_j) = \sum_K a_K(\phi_i, \phi_j),
\]

with

\[
  a_K(\phi_i, \phi_j) = \int_K \nabla \phi_i \nabla \phi_j.
\]

Note that \( a_K(\phi_i, \phi_j) \) is zero unless the nodes \( i \) and \( j \) are both vertices of triangle \( K \). A triangle in the mesh contributes nonzero values to all three vertices with the formula above. Now consider a triangle \( K \) with vertices \( i, j, k \). This triangle has a 3 \( \times \) 3 matrix called the element stiffness matrix:

\[
  A_K = \begin{pmatrix}
    a_K(\phi_i, \phi_i) & a_K(\phi_i, \phi_j) & a_K(\phi_i, \phi_k) \\
    a_K(\phi_j, \phi_i) & a_K(\phi_j, \phi_j) & a_K(\phi_j, \phi_k) \\
    a_K(\phi_k, \phi_i) & a_K(\phi_k, \phi_j) & a_K(\phi_k, \phi_k)
  \end{pmatrix}.
\]

Such a matrix can be made for each triangle in the mesh. Now the matrix \( A \) is made by summing up all contributions \( a_K \) for a certain position in the matrix. This process is called the assembly process. The matrix is computed as

\[
  A = \sum_{e=1}^{n_e} A_e, \quad (4.12)
\]
where $n_e$ is the number of elements. Matrix $A^e$ is of the form

$$A^e = P_e A_{K_e} P_e^T,$$

with $A_{K_e}$ the element stiffness matrix of triangle $K_e$. Matrix $P_e$ is an $n \times 3$ Boolean connectivity matrix, which maps the elements of $A_{K_e}$ to the correct position in $A$. Once this process is completed $AU = b$ can be solved by Gaussian elimination.
Chapter 5

Modelling of a Wastewater Treatment Plant

In this chapter the models describing the motion of a fluid and the model for biological processes in a wastewater treatment plant are combined to one large model. This model can be made with COMSOL Multiphysics 3.5a. A finite element method in COMSOL is used for solving this model. A few models will be discussed.

5.1 Combining ASM with CFD

For the modelling of a wastewater treatment plant a combination of different models can be used. First Activated Sludge Model No. 1 (for other Activated Sludge Models this process works in a similar way) will be used for the modelling of all biological processes in the treatment plant. The transport of the components in ASM1 and thus in the water can be modelled using the convection-diffusion equation. And finally, the flow of the wastewater in a treatment plant can be calculated with the Navier-Stokes equations or a turbulence model.

In chapter 1 Activated Sludge Model is introduced using a mass balance equation,

\[ \text{Accumulation} = \text{Input} - \text{Output} + \text{Reaction}. \]

The reaction terms for this mass balance are given in ASM1. For the modelling mass transport a convection-diffusion equation will be used \[ \text{[11]} \]. This gives the input and output of the mass balance. All concentrations in the wastewater can be modelled in this way. Consider, for example, the concentration of heterotrophic biomass \( X_{BH} \). The complete
mass-balance, after rewriting the equations, will be

\[
\frac{\partial X_{BH}}{\partial t} = \nabla \cdot (k \nabla X_{BH}) - \mathbf{u} \cdot \nabla X_{BH} + \left[ \mu_H \left( \frac{S_S}{K_S + S_S} \right) \frac{S_O}{K_{O,H} + S_O} \right] \eta_g - b_H \]

\[
X_{BH}. \tag{5.1}
\]

For all components in Activated Sludge Model No. 1 an equation similar to 5.1 can be found. Under the assumption that for every component the transport in the water can be described by the convection-diffusion equation, only the reaction terms differ in these equations. These reaction terms can be found in ASM 1. Another example is the equation for autotrophic biomass, given as

\[
\frac{\partial X_{BA}}{\partial t} = \nabla \cdot (k \nabla X_{BA}) - \mathbf{u} \cdot X_{BA} + \left[ \mu \left( \frac{S_{NH}}{K_{NH} + S_{NH}} \right) \frac{S_O}{K_{O,A} + S_O} \right] - b_A \]

\[
X_{BA}. \tag{5.2}
\]

For each component in the wastewater a part of the transport is modelled by convection. Solving the differential equations requires the computation of the velocity vector \( \mathbf{u} \) which contains the velocities for every space direction. For a two dimensional problem \( \mathbf{u} = (u, v) \), with \( u \) the horizontal velocity, and \( v \) the vertical velocity. This velocity can be calculated using the (incompressible) Navier-Stokes equations or a turbulence model. The determination of this velocity vector couples the Activated Sludge Model to a Computational Fluid Dynamics model.

If turbulence is not of great importance, first the Navier-Stokes equations have to be solved. This velocity can be used for solving the complete Activated Sludge Model. If turbulence is needed in the model a turbulence model can be used for solving the velocity.

### 5.2 A Two-dimensional Model

In the previous chapters the Activated Sludge Models and the models for fluid flow are introduced. Now it is time to look at complete model in COMSOL Multiphysics 3.5a. We start with a simple two-dimensional model for a rectangular tank of a wastewater treatment plant. The tank has a length of 100 meter and a depth of 5 meter. The mesh is chosen as a normal sized mesh in COMSOL. There is some scaling applied in vertical direction, in order to get a more equal mesh. The domain and corresponding mesh can be found in figure 5.1.
5.2. A TWO-DIMENSIONAL MODEL

Figure 5.1: A two dimensional representation of a tank of a wastewater treatment plant. It has a length of 100 meter and a depth of 5 meter. A simple COMSOL mesh with triangular elements is chosen.

The flow in this tank is modelled with the incompressible Navier-Stokes equations. For the biological processes Activated Sludge Model No. 1 is used. In appendix A a description can be found for making a model with COMSOL.

5.2.1 Activated Sludge Model No.1

In this model almost all components of ASM1 are modelled. We assume that the alkalinity of the wastewater remains constant at pH = 7. By this assumption the component $S_{ALK}$ in Activated Sludge Model will not be treated. We also assume that the temperature remains constant in the tank at a value of 20 degrees Celsius. All other components like substrate $S_S$ and $X_S$, biomass $X_{B,H}$, $X_{B,A}$ and $X_P$, oxygen $S_O$ and nitrogen components $S_{NO}$, $S_{NH}$, $S_{ND}$ and $X_{ND}$ will be treated. The parameters in ASM1 are chosen equal to the parameters in the article by Henze et al. [8]. The values of the parameters can be found in table 5.1. Because the units of the parameters are different in COMSOL compared with the values in ASM1 a few conversion factors were chosen. For example, mass is given in terms of grams in ASM1, whereas COMSOL Multiphysics uses mol. Take for instance a concentration of oxygen of 5 gram/$m^3$. Using the molar mass of oxygen, $M = 32.00$ g/mol, the oxygen concentration is equal to $5/32.00 \text{ mol}/m^3$. In the model in COMSOL all concentrations will be given in mol/$m^3$.

Two other remarks about the parameters are about the decay rate of autotrophic biomass and the parameter $i_XP$. Both are not given in the table above. We assume that the decay rate of autotrophic biomass is equal to the decay rate of heterotrophic biomass, hence $b_A = b_H$. Further we assume that $i_XP = i_XE$. 
Table 5.1: Parameter values used for implementing ASM1 in COMSOL. All values are valid at a temperature of 20 degrees Celsius and can be found in [8]. All conversion factors used for making consistent units are also in the table.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Y_A$</td>
<td>14.00 - 0.24</td>
<td>dimensionless</td>
</tr>
<tr>
<td>$Y_H$</td>
<td>0.67</td>
<td>dimensionless</td>
</tr>
<tr>
<td>$f_p$</td>
<td>0.08</td>
<td>dimensionless</td>
</tr>
<tr>
<td>$i_{XB}$</td>
<td>0.086</td>
<td>dimensionless</td>
</tr>
<tr>
<td>$i_{XE}$</td>
<td>0.06</td>
<td>dimensionless</td>
</tr>
<tr>
<td>$\mu_H$</td>
<td>6.0</td>
<td>day$^{-1}$</td>
</tr>
<tr>
<td>$K_S$</td>
<td>1 - 20.0</td>
<td>mol/m$^3$</td>
</tr>
<tr>
<td>$K_{O,H}$</td>
<td>0.20</td>
<td>mol/m$^3$</td>
</tr>
<tr>
<td>$K_{NO}$</td>
<td>0.50</td>
<td>mol/m$^3$</td>
</tr>
<tr>
<td>$b_H$</td>
<td>0.62</td>
<td>day$^{-1}$</td>
</tr>
<tr>
<td>$\eta_g$</td>
<td>0.8</td>
<td>dimensionless</td>
</tr>
<tr>
<td>$\eta_h$</td>
<td>0.4</td>
<td>dimensionless</td>
</tr>
<tr>
<td>$k_h$</td>
<td>3.0</td>
<td>day$^{-1}$</td>
</tr>
<tr>
<td>$K_X$</td>
<td>0.03</td>
<td>dimensionless</td>
</tr>
<tr>
<td>$\mu_A$</td>
<td>0.80</td>
<td>day$^{-1}$</td>
</tr>
<tr>
<td>$K_{NH}$</td>
<td>1 - 1.0</td>
<td>mol/m$^3$</td>
</tr>
<tr>
<td>$K_{O,A}$</td>
<td>0.4</td>
<td>mol/m$^3$</td>
</tr>
<tr>
<td>$k_a$</td>
<td>32.00 - 0.08</td>
<td>m$^3$/mol-day</td>
</tr>
</tbody>
</table>

For the initial concentrations of the components in the wastewater a tanks in series model of SIMBA is used. The notation of the components in the model can be found in 5.2. The initial concentration of oxygen is chosen as 5 g/m$^3$.

Table 5.2: Initial concentrations for the components of ASM 1 according to a SIMBA model.

<table>
<thead>
<tr>
<th>Notation</th>
<th>Value</th>
<th>unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ss</td>
<td>27</td>
<td>g COD /m$^3$</td>
</tr>
<tr>
<td>Xs</td>
<td>54</td>
<td>g COD /m$^3$</td>
</tr>
<tr>
<td>Xbh</td>
<td>930</td>
<td>g COD /m$^3$</td>
</tr>
<tr>
<td>Xba</td>
<td>50</td>
<td>g COD /m$^3$</td>
</tr>
<tr>
<td>Xp</td>
<td>750</td>
<td>g COD /m$^3$</td>
</tr>
<tr>
<td>Sno</td>
<td>8.3</td>
<td>g N /m$^3$</td>
</tr>
<tr>
<td>Snh</td>
<td>8.7</td>
<td>g N /m$^3$</td>
</tr>
<tr>
<td>Snd</td>
<td>2.0</td>
<td>g N /m$^3$</td>
</tr>
<tr>
<td>Xnd</td>
<td>1.96</td>
<td>g N /m$^3$</td>
</tr>
</tbody>
</table>

In COMSOL Multiphysics Activated Sludge Model No.1 is modelled using the Convection-
5.2. A TWO-DIMENSIONAL MODEL

Diffusion model of the Chemical Engineering Module. For each component in ASM1 a variable is defined. All parameters and initial concentrations are defined as constants in the model. The rate equations of ASM1 are implemented as global expressions in COMSOL.

The Convection-Diffusion model in COMSOL uses the standard convection-diffusion equation. In the subdomain settings of the model only the diffusion coefficient, reaction terms and velocity for convection have to be defined in order to set up a complete convection-diffusion equation. For ASM1 a diffusion coefficient of 0.01 is chosen, after a few test experiments varying the value of the coefficient. See also Diffusion, mass transfer in fluid systems by E.L. Cussler [4] for more information about diffusion coefficients. For each of the components the reaction terms is set up by the constants and global expressions in COMSOL. Finally the velocities \( \mathbf{u} \) and \( \mathbf{v} \), which is calculated by the incompressible Navier-Stokes equations, is used. It is assumed that for each component in the wastewater the same diffusion coefficient holds.

The Convection-Diffusion model also requires some conditions on the boundaries of the domain. These boundary conditions for the Convection-Diffusion model can be found in table 5.3.

<table>
<thead>
<tr>
<th>Boundary</th>
<th>Condition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Left</td>
<td>Concentration: initial concentration of the component</td>
</tr>
<tr>
<td>Lower</td>
<td>Insulation/Symmetry</td>
</tr>
<tr>
<td>Upper</td>
<td>Insulation/Symmetry</td>
</tr>
<tr>
<td>Right</td>
<td>Convective flux</td>
</tr>
</tbody>
</table>

Table 5.3: Boundary conditions for the Convection-Diffusion model.

5.2.2 The Navier-Stokes Equations

In this two-dimensional model the fluid flow is modelled with the incompressible Navier-Stokes equations. The density of wastewater in the tank is chosen equal to the density of water: \( \rho = 1000 \text{ kg/m}^3 \). The dynamic viscosity in this model is equal to the dynamic viscosity of water \( \mu = 0.001 \text{ Pa}\cdot\text{s} \).

For the Navier-Stokes equations the boundary conditions can be found in table 5.4. At the inlet boundary a parabolic velocity profile is chosen, satisfying the Poiseuille flow. The average velocity is chosen equal to 0.25 m/s. Using a quadratic function a parabolic profile is made, see figure 5.2. The velocity at the bottom is equal to zero, satisfying the no slip condition. Taking the characteristic length of 100 meter for the tank, and the velocity of 0.25 m/s it is possible to calculate the Reynolds number in the tank:

\[
Re = \frac{\rho U L}{\eta} = \frac{1000 \cdot 0.25 \cdot 100}{0.001} = 25 \cdot 10^6.
\]

As we can see \( Re \gg 1 \), so turbulent effects could only appear in a small boundary layer in this case.
5.2.3 Avoiding a Negative Concentration

In some cases the concentration of oxygen can become negative. To avoid a negative concentration, the model can be adjusted with a step function. Once a negative concentration is reached, the concentration of the component is set to zero with this function. In the model a so-called shadow variable given as

\[ C_{\text{shadow}} = \text{flc1hs}(C - 0.1, 0.1) \times C, \]

where \( C \) is the original concentration and \( \text{flc1hs}(x, \text{scale}) \) a stepfunction in COMSOL. Scale defines the interval of the stepfunction: the function is 1 if \( x > \text{scale} \) and zero if \( x < -\text{scale} \), on the interval the smoothed Heaviside function is used by COMSOL. Now, the concentration will be kept the same if it is positive and will be set to zero if it becomes negative.

In the global expressions of this model an additional variable \( \text{So\_lim} \) is introduced as shadow variable for the oxygen concentration. In all process rates the oxygen concentration is replaced by the shadow variable.

5.2.4 Solving the Model

For solving the above model two types of solvers are selected. First, the incompressible Navier-Stokes equations are solved using a stationary solver. A direct solver, called Paradiso is selected, giving the velocities in horizontal and vertical direction \( u, v \) and the pressure \( p \).

Now these velocities are used in solving the Convection-Diffusion model. Here a time-dependent solver is used for a time range from 0 to 5000 seconds. Further, for the BDF method is used for time integration. The size of the time steps is automatically determined by COMSOL and we use the implicit method, the backward Euler method. The results of this model will be discussed in the next chapter.

5.3 A Bubbly-flow Model

The model introduced is a very simple two-dimensional model for a wastewater treatment plant. In this section we will extend the model by using the Bubbly-flow model of COMSOL...
5.3. A BUBBLY-FLOW MODEL

Multiphysics. Using this model makes it possible to add aeration processes to the model of the treatment plant. Also turbulence in the fluid flow can be modelled.

5.3.1 Governing Equations

The Bubbly-flow model is a model with two fluid phases, there is the liquid phase and a gas phase. The model is a simplification of the two-fluid model, based on three assumptions [2]:

- The gas density is negligible compared to the liquid velocity.
- The motion of gas bubbles relative to the liquid is determined by a balance between viscous drag and pressure forces.
- The pressure field is the same for both phases.

The model can be given by a momentum equation for the liquid velocity, a continuity equation and a transport equation for the volume fraction of the gas phase. When turbulence modelling is used, two additional equations are needed. These are the slightly modified equations of the $k - \varepsilon$ turbulence model. The momentum equation of the model is given as

$$
\phi_l \rho_l \frac{\partial \mathbf{u}_l}{\partial t} + \phi_l \rho_l \mathbf{u}_l \cdot \nabla \mathbf{u}_l = -\nabla p + \nabla \left[ \phi_l (\eta_l + \eta_T) \left( \nabla \mathbf{u}_l + \nabla \mathbf{u}_l^T - \frac{2}{3} (\nabla \cdot \mathbf{u}_l) \mathbf{I} \right) \right] + \phi_l \rho_l g + \mathbf{F},
$$

(5.4)

In this equation $\mathbf{u}$ is the velocity vector, $p$ the pressure, $\phi$ the phase volume (fraction), $\rho$ the density, $g$ the gravity vector and $\mathbf{F}$ any additional force. The parameter $\eta$ is the dynamic viscosity and $\eta_T$ the turbulent viscosity. The subscript $l$ denotes that the equation is valid for the liquid phase.

The continuity equation is equal to

$$
\frac{\partial}{\partial t} (\rho_l \phi_l + \rho_g \phi_g) + \nabla \cdot (\rho_l \phi_l \mathbf{u}_l + \rho_g \phi_g \mathbf{u}_g) = 0,
$$

(5.5)

where $g$ denotes the components for the gas phase. By the assumption that the gas density is small and the liquid density is constant, it can be replaced by $\nabla \cdot \mathbf{u}_l = 0$. The last equation is for the transport of the volume fraction of gas and is given by

$$
\frac{\partial \rho_g \phi_g}{\partial t} + \nabla \cdot (\phi_g \rho_g \mathbf{u}_g) = -m_{gl},
$$

(5.6)

where $m_{gl}$ is the mass transfer rate from gas to liquid, see also section 3.2.4.

In COMSOL the velocity for the liquid $\mathbf{u}_l$ is solved. The gas velocity can be calculated with $\mathbf{u}_g = \mathbf{u}_l + \mathbf{u}_{slip} + \mathbf{u}_{drift}$, where $\mathbf{u}_{slip}$ is the relative velocity between the phases and $\mathbf{u}_{drift}$ is an additional contribution for turbulence.

For turbulence modelling the $k - \varepsilon$ model (see section 3.2.2) is used. The transport equation for turbulent kinetic energy is

$$
\rho_l \frac{\partial k}{\partial t} - \nabla \cdot \left[ \left( \frac{\eta + \eta_T}{\sigma_k} \right) \nabla k \right] + \rho_l \mathbf{u}_l \cdot \nabla k = \frac{1}{2} \eta_T \left( \nabla \mathbf{u}_l + (\nabla \mathbf{u}_l)^T \right)^2 - \rho_l \varepsilon + S_k.
$$

(5.7)
The equation for the dissipation of the turbulent kinetic energy becomes

\[ \rho \frac{\partial \varepsilon}{\partial t} - \nabla \cdot \left( \left( \eta + \frac{\eta T}{\sigma_\varepsilon} \right) \nabla \varepsilon \right) + \rho \mathbf{u} \cdot \nabla \varepsilon = \left[ \frac{1}{2} c_1 \eta T \left( \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right)^2 - \rho \right] c_2 \varepsilon + c_3 S_k \varepsilon \]

(5.8)

In these equations \( S_k \) is related to the bubble-induced turbulence and is given by

\[ S_k = -c_k \phi_g \nabla p \cdot \mathbf{u}_{\text{slip}}. \]

The parameters \( c_\varepsilon \) and \( c_k \) should have a value in the following ranges: \( 0.01 < c_k < 1 \) and \( 1 < c_\varepsilon < 1.92 \).

### 5.3.2 Bubbly-flow and ASM1

The model made in COMSOL contains the same two-dimensional domain as the model in the previous section. Again Activated Sludge Model No. 1 is used with parameter values as in table 5.1 and initial concentrations as in table 5.2. Activated Sludge Model No.1 is modelled with the same Convection-Diffusion model. All subdomain settings and boundary conditions are the same as before.

In COMSOL the incompressible Navier-Stokes model is deleted and the bubbly-flow model is added. This model also requires some adjustments to the domain of the model. In order to model the aeration process at the bottom of the tank, the boundary at the bottom is split into three parts. On a small part of this split boundary aeration will be modelled.

The bubbly flow model consists of two phases, liquid and gas. For both phases boundary conditions are needed. The boundary conditions for the liquid phase are similar to the ones for the incompressible Navier-Stokes equations. At the inlet boundary a horizontal velocity is chosen. Because this model also uses turbulence two additional conditions are chosen. The turbulent length scale \( L_T \) is equal to \( 0.07 \times 5 \), where 5 is the height of the tank. The turbulence intensity \( I_T \) is set to 0.1. On the bottom of the tank a logarithmic wall function is chosen and at the top of the tank a slip boundary condition is chosen. At the outlet boundary a hydrostatic pressure is prescribed. A summary of these boundary conditions can be found in table 5.3. Again, the Reynolds number has a value of \( 25 \times 10^6 \), which indicates that turbulent effects can be visible after the obstacle in the flow and in the boundary layer. In this model the gas flux at the bottom can be seen as an obstacle in the flow.
5.3. A BUBBLY-FLOW MODEL

Table 5.5: Boundary conditions for the liquid phase of the bubbly flow model. At the lower boundary \( \delta_w \) is the distance between the real wall and the computational domain [2]. This is also called the displacement thickness [20]. In this condition the distance is given by \( h/2 \), where \( h \) is the grid size. In the outlet condition \( y \) is the variable representing the vertical position in the tank. At the bottom of the tank \( y = 0 \) and at the top of the tank \( y = 5 \).

<table>
<thead>
<tr>
<th>Boundary</th>
<th>Condition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Left</td>
<td>Inlet: Velocity ( u = 0.25 \text{[m/s]} ), ( L_T = 0.07 \times 5 ) and ( I_T = 0.1 )</td>
</tr>
<tr>
<td>Lower</td>
<td>Wall: Logarithmic wall function ( \delta_w = h/2 )</td>
</tr>
<tr>
<td>Upper</td>
<td>Wall: Slip</td>
</tr>
<tr>
<td>Right</td>
<td>Outlet: Pressure ( p = \rho_0 \times 9.81 \text{[m/s}^2]) ( \times (5 - y) )</td>
</tr>
</tbody>
</table>

Table 5.6: Boundary conditions for the gas phase of the bubbly flow model.

<table>
<thead>
<tr>
<th>Boundary</th>
<th>Condition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Left</td>
<td>Gas concentration 0.0</td>
</tr>
<tr>
<td>Lower</td>
<td>Insulation/Symmetry and Gas flux ( 0.01 \times s \times (1 - s) \times 2 )</td>
</tr>
<tr>
<td>Upper</td>
<td>Gas outlet</td>
</tr>
<tr>
<td>Right</td>
<td>Convective flux</td>
</tr>
</tbody>
</table>

For the gas phase also a few boundary conditions are chosen, see table 5.6. In order to prevent a conflict with the inlet boundary for the liquid phase a gas concentration of 0.0 is chosen at boundary 1. At the top of the tank a gas outlet is chosen as boundary condition. At a small part of the bottom the aeration is modelled by adding a gas flux to the tank. It is given a parabolic profile. All other boundaries are chosen as insulation/symmetry.

For the gas flux of the tank also a slip model has to be chosen, which contains information about the gas bubbles, which are blown into the tank. For a wastewater treatment plant we select large spherical bubbles with a bubble diameter of 7e-3 meter. The initial conditions are given for the horizontal velocity and the pressure in the tank.

In the convection-diffusion model, with all equations of Activated Sludge Model No. 1 also two minor changes have to be made. First of all the horizontal and vertical velocity, used in the convection term, need to be changed into the velocities of the liquid (\( u_l \) and \( v_l \)). The bubbly flow model is coupled to the convection-diffusion model by the diffusion coefficient. The diffusion coefficient is given by

\[
D = \frac{\eta_T}{\rho_l}, \quad (5.9)
\]

where \( \eta_T \) is the turbulent viscosity from the bubbly flow model and \( \rho_l \) the density of the wastewater [2].
5.3.3 Solving the Model

Solving the bubbly-flow model requires some adjustments of the mesh. Because the flow becomes turbulent a boundary layer mesh in COMSOL is used. The mesh is chosen to be fine and at the gas inlet at the bottom of the tank, the mesh is chosen even finer.

The bubbly flow model is still solved with a stationary solver, but the variables are split into two segregated groups. The first group contains variables like velocity and pressure. The second group contains logarithmic terms, which are needed in the turbulence modelling. The segregated stationary solver of COMSOL is used, where we still have selected the direct Paradiso solver. In order to make sure that a solution is found, weak constraints are used in the model, giving additional variables in the segregated group.

The convection-diffusion model is still solved with a time-dependent solver, with a time range from 0 to 5000 seconds. In this case a segregated time-dependent solver is used. Again the BDF method is used for time integration. The backward Euler method is still together with automatic time stepping.

5.4 A Bubbly-flow Model with Mass Transfer

This model shows an extension of the bubbly flow model in the previous section. Mass transfer is added in order to give a more realistic model for the aeration process in the tank.

It is assumed that oxygen is only added into the tank by the aeration process. During this process, air (which contains 20 % oxygen) is blown into the tank. The bubbly-flow model introduced in the previous section is used. In the subdomain settings of the model mass transfer can be selected. The mass transfer is modelled with the two film theory, which is introduced in section 3.2.4. The mass transfer coefficient is chosen to be 0.001. Furthermore Henry’s constant is needed. This constant is determined for all types of gases. Henry’s constant is a temperature dependent constant and is also called Henry’s coefficient. For a lower temperature the amount of oxygen dissolved in the water becomes higher. For out model we use the value of Henry’s constant for oxygen, which is \(7.8 \cdot 10^4\) Pa\(\cdot\)m\(^3\)/mol.

The concentration component added for mass transfer is given with an convection-diffusion equation. This concentration contains the amount of mass which is added from mass transfer of the gas flux. Mass transfer is given in COMSOL by a reaction term, which is given as the mass transport from gas to liquid of the bubbly flow model divided by the molar mass of the gas:

\[
R = \frac{m_{\text{g}}}{M}. \tag{5.10}
\]

In the tank of a wastewater treatment plant we are interested in the amount of oxygen. The reaction term of mass transfer is added to the convection diffusion model for the oxygen concentration of Activated Sludge Model No. 1. All other subdomain settings and boundary conditions are as before. The total equation for the oxygen concentration in
ASM1 becomes
\[
\frac{\partial S_O}{\partial t} = \nabla \cdot (k \nabla S_O) - \mathbf{u} \cdot \nabla S_O
\]
\[\begin{align*}
&- \frac{1 - Y_H}{Y_H} \mu_H \left( \frac{S_S}{K_S + S_S} \right) \left( \frac{S_O}{K_{O,H} + S_O} \right) X_{BH} \\
&- \frac{4.57 - Y_A}{Y_A} \mu_A \left( \frac{S_{NH}}{K_{NH} + S_{NH}} \right) \left( \frac{S_O}{K_{O,A} + S_O} \right) X_{BA} + \frac{m_{gl}}{M}.
\end{align*}\]

All other components of Activated Sludge Model No. 1 are modelled in the same way as before. The boundary conditions are equal to the ones in the previous model. The Reynolds number is still much larger than 1, so turbulent effects may appear behind the aerated part of the tank and in a very small boundary layer.

In order to solve the model without any errors (due to memory shortage of the computer) in COMSOL Multiphysics, we now look at a slightly smaller activated sludge tank. The tank has a length of 75 meters and a height of 4 meters. The bottom of the tank is again split into three parts, see also figure 5.3. The first two parts of this boundary both have a length of 7.5 meters. The remaining part of the boundary is 60 meters. The aeration process is modelled using a gas flux as boundary condition on the second part of the lower boundary. For the two remaining parts an Insulation/Symmetry condition is used as boundary condition, see also tables 5.5 and 5.6.

### 5.4.1 Solving the Model

For solving the model, first the mesh is made. In this model a boundary mesh is used. The density of the mesh is chosen to be fine. The mesh is refined at the boundary where the gas flux is given. The domain and mesh can be found in figure 5.3.

![Figure 5.3: Domain and mesh for the bubbly flow model with mass transfer. The red arrow shows the aerated part of the bottom of the tank. The mesh is chosen finer at this part.](a) Domain (b) Mesh)

We are going to solve this model in three steps. First the bubbly flow is solved with a stationary segregated solver. For solving we use weak constraints. Bubbly flow is solved, except for the bubble density, using the direct PARADISO solver. Next the bubble density is stationary solved. And finally we solve the Activated Sludge Model No.1 together with
the effective density in the tank with a time-dependent solver. The results of the model can be found in the next chapter.
Chapter 6

Results of the Numerical Models

In the previous chapter a few models were introduced describing the hydraulic and biological processes in a wastewater treatment plant. This chapter gives a description of the results of these models.

6.1 Expectations

Before we start with a discussion of the results, first some expectations are treated. We expect that an aeration process in the tank has quite some influence on the fluid flow. The flow can get a turbulent character, because the gasflux used for the aeration process is an obstacle in the fluid flow. This also means that so-called dead zones could arise in the tank. In a tank without aeration the flow will probably be laminar.

In Activated Sludge model No. 1 all processes depend on each other forming one large system. One of the difficulties of the model is to see what happens with the concentrations. Based on the fact that we want to remove pollution from the wastewater and by looking closely to the process, some expectations about the model can be formulated.

We expect to see a growth of heterotrophic biomass in the tank, under the assumption that the decay is smaller than the growth. The biomass grows aerobically using soluble substrate, ammonia and oxygen. The concentrations of these components should decrease. The hydrolysis of particulate substrate into soluble substrate gives a lower concentration for particulate substrate.

For the growth of autotrophic biomass there are some differences. Again under the assumption that growth is larger than decay, we expect to see an increasing concentration of biomass. For the process ammonia and oxygen are used, implying that both concentrations should decrease in the tank. In the nitrification process nitrate is formed, resulting in an increasing concentration of nitrate. Nitrate is used together with soluble substrate for the anoxic growth of heterotrophic biomass. Therefore the nitrogen concentration should decrease in the tank.
The decay of biomass gives a small increase in the concentration of decay material and particulate substrate. For the first one we expect to see the concentration to increase in the results, while the latter is transformed into soluble substrate giving a decrease of the concentration.

For the particulate biodegradable nitrogen the concentration should decrease. In the decay process of biomass particulate biodegradable nitrogen is formed. This is followed by an hydrolysis process, which transforms the nitrogen into soluble biodegradable nitrogen. A decrease of concentration is expected for this component, under the assumption that hydrolysis has more influence. The soluble nitrogen is transformed into ammonia, which is used for the growth of biomass. We expect that the concentration in the tank decreases.

### 6.2 A Two-dimensional Model

First, consider the results of the simple two-dimensional model of a tank in a wastewater treatment plant. In this section some of the results are presented and discussed. First we start with the velocity of the fluid in the tank. Figure 6.1 contains the velocity field in the tank. Also a few streamlines of the flow in the tank are drawn. The figure shows a laminar flow. The velocity satisfies the no-slip condition at the bottom of the tank, where the velocity is zero. The maximum velocity of the fluid flow can be found at the top of the tank, just as prescribed by the parabolic profile (Poiseuille flow) of the inlet boundary condition.

![Velocity field and some streamlines in the tank of a treatment plant.](image)

The figures 6.2, 6.3, and 6.4 show the distribution of the components of Activated Sludge Model No. 1 in the tank. In table 6.1 the maximum and minimum concentrations for each component in the model are given.
6.2. A TWO-DIMENSIONAL MODEL

(a) Soluble substrate

(b) Particulate substrate

(c) Heterotrophic biomass

(d) Autotrophic biomass

Figure 6.2: Distribution of substrate and biomass in the tank. Concentrations are plotted.
CHAPTER 6. RESULTS OF THE NUMERICAL MODELS

Figure 6.3: Distribution of all nitrogen components in the tank. Concentrations are plotted.
6.2. A TWO-DIMENSIONAL MODEL

(a) Decay material

(b) Dissolved oxygen

Figure 6.4: Distribution of decay material and dissolved oxygen in the tank. Concentrations are plotted.

<table>
<thead>
<tr>
<th>Component</th>
<th>Minimum</th>
<th>Maximum</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soluble substrate (Ss)</td>
<td>13.84</td>
<td>27.00</td>
</tr>
<tr>
<td>Particulate substrate (Xs)</td>
<td>51.36</td>
<td>54.00</td>
</tr>
<tr>
<td>Heterotrophic biomass (Xbh)</td>
<td>930.00</td>
<td>939.46</td>
</tr>
<tr>
<td>Autotrophic biomass (Xba)</td>
<td>49.88</td>
<td>50.00</td>
</tr>
<tr>
<td>Particulate substrate (Xp)</td>
<td>750.00</td>
<td>750.27</td>
</tr>
<tr>
<td>Dissolved oxygen (So)</td>
<td>0.48</td>
<td>5.00</td>
</tr>
<tr>
<td>Nitrate nitrogen (Sno)</td>
<td>7.93</td>
<td>8.41</td>
</tr>
<tr>
<td>Ammonia nitrogen (Snh)</td>
<td>8.13</td>
<td>8.70</td>
</tr>
<tr>
<td>Soluble biode. nitrogen (Snd)</td>
<td>1.51</td>
<td>2.00</td>
</tr>
<tr>
<td>Particulate biode. nitrogen (Xnd)</td>
<td>1.94</td>
<td>2.00</td>
</tr>
</tbody>
</table>

Table 6.1: Minimum and maximum concentrations for each of the component in the tank. All concentrations are in $g/m^3 = mg/l$.

Due to the fluid flow the components in the wastewater are transported in the tank. The distribution of components in the wastewater is influenced by this flow. In the figures 6.2, 6.3 and 6.4, the effects can be found. The parabolic profile of the velocity also appears in the distribution of the concentrations in the tank. Take, for example, the concentration of
soluble substrate in figure 6.2(a). At the inlet on the left side of the tank the concentration is higher compared with the outlet, just as expected. The influence of the velocity is also visible. The substrate concentration remains higher at the top of the tank. Due to the higher velocity a larger amount of the material is transported to that part of the tank. This holds for all wastewater components with decreasing concentration. For components with an increasing concentration, for example the heterotrophic biomass (figure 6.2(c)), a similar effect is visible.

Next, we look to the concentrations of the components in table 6.1 together with their distributions in the tank. The concentrations of the particulate and soluble substrate decrease in the tank, just as expected. The heterotrophic biomass shows indeed a growth in the tank. The concentration autotrophic biomass decreases. This is not exactly what we would expect. The concentration of decay material in the tank remains more or less constant, while we would like to see an increase of the concentration.

For the concentrations of nitrogen the results are a bit disappointing. The differences between the maximum and minimum concentration in the tank are small. The wastewater is not completely cleaned from its pollution. The distributions in the tank satisfy our expectations. The concentrations of ammonia, nitrate and soluble biodegradable nitrogen decrease in the tank. The concentration of particulate biodegradable nitrogen shows a small increase of the concentration. There are two possible reasons for these results. First of all, there could be a shortage of oxygen in the tank. In most processes in Activated Sludge Model No. 1 oxygen is used. It could be that all oxygen is already used for the aerobic growth of heterotrophic biomass. This means there is too little oxygen left for all other processes. Maybe the oxygen concentration of 5 mg/l is too low to give reasonable results. Another reason for these results could be the choice of initial concentrations for the components in the wastewater. The concentration of activated sludge (heterotrophic and autotrophic biomass, decay material) is quite low. A higher concentration of sludge implies more activity in the tank. This means that the concentrations of the pollution (substrate and nitrogen components) will probably show a larger decrease.

With COMSOL it is also possible to plot the concentration at the outlet against time. For the most interesting components (soluble substrate, heterotrophic biomass, dissolved oxygen and nitrate) such a plot at the middle of the outlet can be found in the figures 6.5 and 6.6. Looking at all four figures we see that Activated Sludge Model No. 1 reaches a stationary solution. Also the concentrations behave as expected. Heterotrophic biomass grows and the concentrations of soluble substrate and oxygen decrease. The concentration of nitrate first grows a bit, due to the growth of autotrophic biomass, then decreases because it is used for the growth of heterotrophs.
6.2. A TWO-DIMENSIONAL MODEL

Figure 6.5: Concentrations against time at the outlet of the tank.

(a) Soluble substrate  
(b) Heterotrophic biomass

Figure 6.6: Concentrations against time at the outlet of the tank.

(a) Dissolved oxygen  
(b) Nitrate
6.2.1 Changing the Growth Parameters

In the previous model all constants were equal to the ones determined by Henze et al. Here the values of the growth parameters are changed, just as in the article by Huang, Wu, Xiao and Xia. In this article Activated Sludge Model No. 1 is coupled to a CFD package called FLUENT. In their research they found that the growth parameters of heterotrophic biomass $\mu_H$ and autotrophic biomass $\mu_A$ should be much larger compared with the original ones. The values are chosen as 50.0 for the heterotrophic biomass and 8.0 for the autotrophic biomass. All other model components, including the other parameter values, are kept the same. Again an oxygen concentration of 5 mg/l is used.

The velocity field is still the same with a parabolic profile and can be found in figure 6.1. The distributions of the components are given in the figures 6.7. The minimum and maximum concentrations are given in table 6.2.

<table>
<thead>
<tr>
<th>Component</th>
<th>Minimum</th>
<th>Maximum</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soluble substrate</td>
<td>0.27</td>
<td>27.00</td>
</tr>
<tr>
<td>Particulate substrate</td>
<td>53.17</td>
<td>54.00</td>
</tr>
<tr>
<td>Heterotrophic biomass</td>
<td>930.00</td>
<td>947.58</td>
</tr>
<tr>
<td>Autotrophic biomass</td>
<td>49.88</td>
<td>50.00</td>
</tr>
<tr>
<td>Decay material</td>
<td>750.00</td>
<td>750.27</td>
</tr>
<tr>
<td>Dissolved oxygen</td>
<td>-0.70</td>
<td>5.00</td>
</tr>
<tr>
<td>Nitrate nitrogen</td>
<td>7.30</td>
<td>8.55</td>
</tr>
<tr>
<td>Ammonia nitrogen</td>
<td>7.04</td>
<td>8.70</td>
</tr>
<tr>
<td>Soluble biode. nitrogen</td>
<td>1.45</td>
<td>2.00</td>
</tr>
<tr>
<td>Particulate biode. nitrogen</td>
<td>1.94</td>
<td>2.00</td>
</tr>
</tbody>
</table>

Table 6.2: Minimum and maximum concentrations for each of the component in the tank. All concentrations are in g/m$^3$, which is the same as mg/l.
6.2. A TWO-DIMENSIONAL MODEL

(a) Soluble substrate
(b) Particulate substrate
(c) Heterotrophic biomass
(d) Autotrophic biomass
(e) Nitrate nitrogen
(f) Ammonia nitrogen
(g) Soluble biodegradable nitrogen
(h) Particulate biodegradable nitrogen
(i) Decay material
(j) Dissolved oxygen

Figure 6.7: Distribution of all concentrations of the components of ASM 1 in the tank.

Looking at the results made with larger growth parameters show some interesting things. First, the oxygen concentration in the tank, it decreases quite fast in the first (left) part of the tank. In the previous model we saw that oxygen was distributed in the complete tank. The minimum oxygen concentration is of the same order as before. The distribution tells us that the oxygen is completely used in the first part of the tank, meaning that the processes will come to an end in the rest of the tank. This is not a desired situation. The concentration of soluble substrate becomes a factor 10 smaller compared with the model with the original growth parameters, compare the concentrations $S_s$ in tables 6.1 and 6.2. This could be an improvement in the model, because we want the concentration substrate in the wastewater as low as possible.

The particulate substrate concentration is larger compared with the previous model.
CHAPTER 6. RESULTS OF THE NUMERICAL MODELS

This is caused by a larger amount of decay material, which is transformed into particulate substrate. In this case the original values of the growth parameters might be better, because it gives a lower concentration. The concentration of heterotrophic biomass grows a bit more in this model. Of course, this is something we would expect, since the growth parameter is larger. However, the difference between the minimum and maximum concentration of autotrophic biomass remains small. We would expect more growth of autotrophic biomass according to the larger growth parameter. This result shows that influence of the growth parameter on autotrophic biomass is not very large.

Comparing all results of the nitrogen components (nitrate, ammonia, soluble and particulate biodegradable nitrogen), there is very little variation in the results. The minimum and maximum concentrations have more or less the same value. This implies that the values of the growth parameters have little influence on the concentrations with nitrate. Another reason could be the low oxygen concentration. Perhaps the processes are ended because all oxygen is already used in the growth processes of biomass.

In general we can say that a larger value for the growth parameters does not improve the model a lot. The results show no important improvements. It could be useful to tweak these parameters in order to make the results more realistic. Perhaps a higher oxygen concentration in the model gives better results.

6.3 A Bubbly-flow Model

The second model made for an activated sludge tank uses the bubbly flow model of COMSOL. Not only fluid flow is of importance in this model but also the transport gas is modelled. This means that the aeration in the tank can be modelled. In figure 6.8 the influence of the gas flux on the fluid flow can be seen. Due to the gas flux the velocity of the fluid increase at the point where the gas enters the tank. After this point the fluid velocity is low. The velocity is also low at the top of the tank. These are the so-called dead zones in the tank. Away from the aeration point the fluid flow becomes laminar. The distributions for the components in Activated Sludge Model No. 1 can be found in figure 6.9. The minimum and maximum concentrations in the tank can be found in table 6.3 and a selection of concentrations against time are given in figure 6.10.

Figure 6.8: Velocity field in the tank. We can see the influence of aeration on the flow.
6.3. A BUBBLY-FLOW MODEL

(a) Soluble substrate
(b) Particulate substrate
(c) Heterotrophic biomass
(d) Autotrophic biomass
(e) Nitrate nitrogen
(f) Ammonia nitrogen
(g) Soluble biodegradable nitrogen
(h) Particulate biodegradable nitrogen
(i) Decay material
(j) Dissolved oxygen

Figure 6.9: Distribution of substrate and biomass in the tank. Concentrations are plotted.
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Figure 6.10: Concentrations against time at the outlet of the tank.
6.4. A BUBBLY-FLOW MODEL WITH MASS TRANSFER

<table>
<thead>
<tr>
<th>Component</th>
<th>Minimum</th>
<th>Maximum</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soluble substrate</td>
<td>15.41</td>
<td>27.00</td>
</tr>
<tr>
<td>Particulate substrate</td>
<td>51.49</td>
<td>54.00</td>
</tr>
<tr>
<td>Heterotrophic biomass</td>
<td>930.00</td>
<td>938.50</td>
</tr>
<tr>
<td>Autotrophic biomass</td>
<td>49.90</td>
<td>50.00</td>
</tr>
<tr>
<td>Decay material</td>
<td>750.00</td>
<td>750.23</td>
</tr>
<tr>
<td>Dissolved oxygen</td>
<td>0.50</td>
<td>5.00</td>
</tr>
<tr>
<td>Nitrate nitrogen</td>
<td>8.03</td>
<td>8.41</td>
</tr>
<tr>
<td>Ammonia nitrogen</td>
<td>8.16</td>
<td>8.70</td>
</tr>
<tr>
<td>Soluble biode. nitrogen</td>
<td>1.58</td>
<td>2.00</td>
</tr>
<tr>
<td>Particulate biode. nitrogen</td>
<td>1.94</td>
<td>1.99</td>
</tr>
</tbody>
</table>

Table 6.3: Minimum and maximum concentrations for each of the component in the tank. All concentrations are in g/m$^3$, which is the same as mg/l.

Looking at the distribution of the concentrations in the tank we see something strange. It looks like the velocity does not influence the distribution of the concentration at all and that the concentration differences are only due to diffusion. This is probably not what we would expect to see in the tank. Checking the model did not show any errors. The concentrations plotted against time show again a stationary solution for ASM1. A possible explanation for these can be found in the use of the bubbly flow model. In the model the fluid flow is calculated with a turbulence model. The components in the wastewater are mixed due to this turbulence. The influence of the fluid flow on the distribution of the components in the tank is therefore quite small. This is also caused by the homogeneous inflow of oxygen in the tank.

Comparing the minimum and maximum concentrations in the tank with the ones found in the previous model, we see that the values are more or less the same. So both models, with the incompressible Navier-Stokes equations and bubbly flow model for fluid flow, give the same results for Activated Sludge Model No. 1. However, the distribution of the concentrations in the tank is quite different.

Although the results above are a bit disappointing, the bubbly flow model of COMSOL Multiphysics is most suitable for modelling the activated sludge tank with an aeration process. In the next section the results of the bubbly flow model with mass transfer will be treated. We will see these are quite promising.

6.4 A Bubbly-flow Model with Mass Transfer

The bubbly flow model is extended with mass transfer for oxygen. Air enters the tank with an aeration process and we assume that the oxygen dissolves into the water. Due to computational problems the chosen tank is a bit smaller compared with the previous models. Again we first look at the velocity field in the tank, which can be found in figure
The influence of the aeration process to fluid flow in the tank is more or less the same as in the previous model. The velocity becomes higher at the bottom of the tank where the aeration process is modelled. Right after this part, the velocity is low and a dead zone arises. We see a similar effect at the top of tank. We could say that the fluid flow gets a turbulent character, in that part of the tank, where the aeration process is modelled. In the remaining parts the fluid flow is laminar.

For calculating the mass transfer of oxygen in the model, COMSOL Multiphysics calculates the interfacial area between the gas and liquid phase. This area is calculated with the number of bubbles in the tank. In figure 6.12 the bubble density can be found. The maximum number of bubbles is 45870 per m$^3$.

Again we are going to look at the concentrations of the components of ASM1 in the tank. These can be found in the figures 6.13, 6.14 and 6.15. The minimum and maximum concentration for each component are given in table 6.4. Finally the most interesting components are plotted against time in the figures 6.16 and 6.17.
6.4. A BUBBLY-FLOW MODEL WITH MASS TRANSFER

Figure 6.13: Distribution of substrate and biomass in the tank. Concentrations are plotted.
CHAPTER 6. RESULTS OF THE NUMERICAL MODELS

(a) Nitrate nitrogen

(b) Ammonia nitrogen

(c) Soluble biodegradable nitrogen

(d) Particulate biodegradable nitrogen

Figure 6.14: Distribution of all nitrogen components in the tank. Concentrations are plotted.
6.4. A BUBBLY-FLOW MODEL WITH MASS TRANSFER

Figure 6.15: Distribution of decay material and dissolved oxygen in the tank. Concentrations are plotted.
CHAPTER 6. RESULTS OF THE NUMERICAL MODELS

(a) Soluble substrate
(b) Heterotrophic biomass

Figure 6.16: Concentrations against time at the outlet of the tank.

(a) Dissolved oxygen
(b) Nitrate

Figure 6.17: Concentrations against time at the outlet of the tank.
First we look at the concentrations plotted against time at the outlet of the tank. Because large time steps were taken for the output in COMSOL, the graphs are not very smooth. Again we see that ASM1 converges to a stationary solution in time. Looking at the dissolved oxygen concentration against time it looks like the concentration increases. This is not completely true, the concentration increases because the initial concentration was zero, but oxygen is still used in the tank. This can be found in the figures 6.15(b) and 6.18.

![Graph of dissolved oxygen concentration against time at the outlet of the tank.](image)

Figure 6.18: Oxygen concentration at the aerated part of the tank (blue) and at the end of the tank (green). Because the initial concentration of oxygen is zero, the concentration increases. Oxygen is also used in the process, giving a lower concentration at the end of the tank.
Looking at the distribution of the concentrations in the tank, than we can see the influence of the aeration process with mass transfer. The concentration of substrate decreases from the aerated part to the end of the tank. We also see that the heterotrophic biomass grows in this way. The concentration autotrophic biomass remains more or less constant, showing a very small decrease in concentration. The concentration differences at the left (inlet) and right (outlet) side of the tank are again small for the nitrogen components. Most concentration satisfy the expectations about growth and decay.

Comparing the minimum and maximum concentrations in table 6.4 with the values found in the previous models we see that the values are more or less the same for each model. This is not very surprising, because the same Activated Sludge Model is solved, with the same initial and parameter values. The distribution of the concentration of each component is quite different if we compare it with the previous models.

Two final remarks about these results are also made for the previous model. First of all, the concentration of oxygen might be too low. Not all processes in ASM1 may work in an optimal way. Second, are the initial concentrations. Although they were taken from a SIMBA model, they might not work for the chosen tank in the COMSOL model.
Chapter 7

Conclusion and Discussion

7.1 Conclusions

‘Is it possible to combine an Activated Sludge Model with Computational Fluid Dynamics?’ is the main subject of this thesis. An Activated Sludge Model describes a few biological processes, which are used in a wastewater treatment plant for cleaning the water. The basis of the model are mass-balance equations for each of the components in the wastewater, for example substrate and biomass. In these equations the mass transport can be modelled using a convection-diffusion equation. Together with the reaction terms of Activated Sludge Model No. 1, the total set of mass-balances can be given.

In the tank of a treatment plant the fluid flow can be calculated using Computational Fluid Dynamics. The incompressible Navier-Stokes equations can be used. If the flow becomes turbulent it is also possible to use a turbulence model, for instance the $k - \varepsilon$ model. In some parts of the tank of a real wastewater treatment plant an aeration process is used to add oxygen to the system. This oxygen is used in the biological processes. The effects of aeration on the fluid flow can be modelled with a bubbly flow model.

It turns out that both described models, ASM1 and a fluid flow model, can be coupled with each other. Therefore it is necessary to first solve the fluid flow model from CFD. We compute the liquid velocity in the tank. This velocity can be used in the convective term of the total mass-balance of Activated Sludge Model No. 1. If the flow becomes turbulent a second coupling between the models arises. In the fluid flow model the turbulent viscosity is calculated. This is used to determine the diffusion coefficient in Activated Sludge Model No. 1. The diffusion coefficient is given by the turbulent viscosity divided by the liquid density.

A third coupling between ASM1 and CFD arises when mass transfer is used. In the bubbly flow model of COMSOL Multiphysics 3.5a mass transfer can be calculated. This is directly coupled to a concentration in the convection-diffusion model. In the case of ASM1 this is oxygen. The reaction term in the mass-balance is extended with an additional term
describing the mass transfer.

Because of the complexity of Activated Sludge Model No.1 it was unfortunately not possible to simplify the model. Only the alkalinity of the wastewater could be omitted. All reaction terms depend on each other making it impossible to reduce the model size.

During the research a few two-dimensional models in COMSOL Multiphysics are made, in which ASM1 is coupled to a CFD model. First, a simple model with the incompressible Navier-Stokes is treated. The results show that both models can be coupled. In the second model the fluid flow is modelled with the more realistic bubbly flow model, where also an aeration process is introduced. Still the coupling between the models work. The last model in COMSOL is an extension of the bubbly flow model with mass transfer. This is the most realistic model for the activated sludge tank of a wastewater treatment plant. We see in the results that the aeration process influences the fluid flow, giving the flow a turbulent character. Also the distribution of the concentrations satisfy most of the expectations.

7.2 Discussion

In theory the coupling between Activated Sludge Model No. 1 and the incompressible Navier-Stokes equations or the bubbly flow model works fine. In practice there are a few points of discussion. First of all the models presented in this thesis are only two dimensional. This is a major simplification of the real world. In the models the tank of a wastewater treatment plant is considered as a rectangle. In a real treatment plant the tank will be a cylinder or the shape of a U. This has quite a large influence on the fluid flow. Also turbulence modelling is quite difficult in two dimensions. A three dimensional model would be more realistic.

The results we have seen in the models are not very realistic. This especially hold for the autotrophic biomass, which should grow, and the nitrogen components which concentrations should decrease. The concentration of the first one decreases in the models and the differences in concentrations of the latter are very small. There are probably two reasons for these results. First, there is the amount of oxygen available for the processes. Maybe the concentration is too low, for the optimal performance of Activated Sludge Model No. 1. All oxygen may already be used for one process (for example the growth of heterotrophs) causing a shortage of oxygen for all other processes. Perhaps the length at the bottom of the tank, where the aeration process is modelled, is too short. Resulting in a low amount of air inserted into the tank. A third reason could be the choice of initial concentrations for the components in the wastewater and the activated sludge. Especially the initial concentration of activated sludge has quite some influence on the combined model.

Finally, we arrive at the benefits and drawbacks of combination of Activated Sludge Model No.1 and a fluid flow model from Computational Fluid Dynamics. One of the major benefits is the more realistic and accurate modelling of the fluid flow in the tank. It is not necessary to model the flow with a tanks-in-series model, but a complete turbulent
flow can be calculated. This also improves the results for the concentrations in the tank. In a tanks-in-series model only inlet and outlet concentrations can be found. With the combined model also the distributions of components (the concentration) in the tank are calculated by approximation.

Of course, there are also some drawbacks about the combined model. Activated Sludge Model No.1 is a complex model with a lot of parameters. It is quite difficult to find the right values for these parameters. Also the influence of input concentrations is of importance. It is necessary to find good initial values. A final drawback is the computational power of the computer. The combined model is quite large and is solved in two or three steps. Memory shortage can occur during the calculation, making it impossible to solve the model.

7.3 Recommendations for Further Work

Unfortunately, it was not possible to answer all questions introduced in chapter 1 in the given amount of time for this project. For the same reason, some discussion points above are not yet tackled. Some recommendations for further work are the following:

- The first recommendation for improving the combined model is to calibrate and validate the model. Based on measurements of concentrations in a real wastewater treatment plant, try to find initial concentrations for the components in the wastewater and the activated sludge. It is also possible to make a model of the real treatment plant in SIMBA and use this information in the COMSOL model. Because the concentrations in the wastewater (at the beginning and end of the tank) are known from the measurements, it is easy to validate the model.

- Investigate the influence of a higher or lower oxygen concentration. If possible, try to improve the mass transfer in the model. Does the autotrophic biomass still decrease? Are the effects on the nitrogen components larger?

- All parameter values are chosen from the literature. Further research is needed to find out whether or not the combined model of CFD and ASM needs different parameter values compared with the tanks-in-series model. Maybe it is possible to find other values for the parameters in the literature. If not, small variations on the existing parameters might also improve the results. In that case it is necessary to compare the results of the combined model with measurements of a real wastewater treatment plant or with a tanks-in-series model. The results of the combined model and the tanks-in-series model should be more or less the same, and fit the measurements of an existing treatment plant.

- Extend the model to a three-dimensional model. The fluid flow becomes more realistic in this case. The same equations in this thesis for ASM1 and CFD are still valid in three dimensions. This requires a computer which has enough memory available. First the fluid flow can be solved. Followed by a computation solving Activated
Sludge Model No. 1 in smaller blocks of the tank. The results of this model will be much more realistic compared with the two dimensional models.

- Extend Activated Sludge Model No. 1 to Activated Sludge Model No. 2 or Activated Sludge Model No. 2d in the CFD-ASM model in COMSOL Multiphysics. This adds the processes of the removal of phosphorus to model, making it more realistic. Also the influence of the temperature on the processes can be investigated with Activated Sludge Model No. 2(d).
Appendix A

How to make a Model with COMSOL Multiphysics

In this appendix a short step by step description is given to set up a model in COMSOL Multiphysics 3.5a. See also the Model Library of COMSOL Multiphysics \[2\] for more details.

Choosing the Model

1. In the Model Navigator (figure A.1) go to Space dimension and select 2D.

Figure A.1: Model Navigator of COMSOL Multiphysics 3.5a.
2. Select Chemical Engineering Module > Momentum Transport > Laminar Flow > Incompressible Navier-Stokes.
3. Click the Multiphysics button followed by Add.
5. In the dependent variables field fill in Ss, Xs, Xbh, Xba, Xp, So, Sno, Snh, Sn and Xnd followed by Add.
6. Click OK.

Constants and Global Expressions
1. Go to Options and select Constants.
2. Fill in the table with the constants and initial values as mentioned in section 5.2. For example the density, type for the name rho in the first column. In the second column type the value 1000 [kg/m³]. For each constant the unit can be given between the brackets [ ].
3. Click OK.
4. Again go to Options and select Expressions > Global Expressions.
5. Fill in the rate equations of Activated Sludge Model No. 1 as global expressions. Defined constants in COMSOL can be used. The variables of the rate equations are already defined when the model was selected. Name the equations r1, r2,..., r10.
6. Define a shadow variable for the oxygen concentration So,lim with a stepfunction: \( f_{\text{c1hs}}(So - 0.1, 0.1) \cdot So \).
7. Click OK.

Drawing the Domain
1. Go to the Draw menu and select Specify Objects > Rectangle.
2. In the window that appears fill in 50 for x and 5 for y. Click OK.
3. Repeat the two steps above and add a x-displacement by filling in position x with the value 50. Click OK.
4. Go to Options > Axes/Grid Settings.
5. Turn off the Axis equal. Fill in the following numbers: x min -5, x max 105, y min -5 and y max 15. Click OK.

Physical Settings
1. Go to the Multiphysics menu and select Convection-Diffusion.
2. Go to the **Physics** menu and select **Subdomain Settings** (figure A.2).

![Figure A.2: Window of COMSOL for the subdomain settings.](image)

3. Select both subdomains by clicking 1 and 2 while holding the *Ctrl* key.
4. Fill in the fields **D (isotropic)**, **u** and **v** with respectively 0.01, **u** and **v**. Also fill in the edit field **R** with the reaction equation (consisting of constants and rate equations) of Activated Sludge Model No.1 for the component. Repeat this for all components.
5. Go to the **Init** tab and fill in all initial conditions, which are defined as constants. Click **OK**.
6. Go to the **Physics** menu and select **Boundary Settings** (figure A.3).

![Figure A.3: Window of COMSOL for the boundary conditions.](image)
7. Select boundary 1 and choose Concentration. Give it the value of the initial concentration. Select boundary 7. Change it into Convective Flux. Select all other boundaries and choose Insulation/Symmetry. Repeat this for each component in the model. Finally, click OK.

8. Go to the Multiphysics menu and select Incompressible Navier-Stokes.

9. Repeat the steps 3 to 7 for the Navier-Stokes equations. For the Subdomain Settings information can be found in table A.1. Boundary conditions are in table A.2.

<table>
<thead>
<tr>
<th>Variable</th>
<th>( \rho )</th>
<th>( \eta )</th>
<th>Initial value ( u )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \rho )</td>
<td>rho</td>
<td></td>
<td>0.25 ( \text{[m/s]} ) *(y/5) *(2 - (y/5))</td>
</tr>
<tr>
<td>( \eta )</td>
<td>eta</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table A.1: Subdomain settings for the incompressible Navier-Stokes equations.

<table>
<thead>
<tr>
<th>Boundary</th>
<th>Condition</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Inlet: Velocity ( u ) 0.25 ( \text{[m/s]} ) *(y/5) *(2 - (y/5))</td>
</tr>
<tr>
<td>3,6</td>
<td>Wall: No slip</td>
</tr>
<tr>
<td>2,5</td>
<td>Wall: Slip</td>
</tr>
<tr>
<td>7</td>
<td>Outlet: No viscous stress, ( p_0 = 0 )</td>
</tr>
</tbody>
</table>

Table A.2: Boundary conditions for the incompressible Navier-Stokes equations.

10. Click OK.

Mesh and Solver

1. Go to the Mesh menu and select Free Mesh Parameters.
2. For the Predefined mesh sizes select Fine.
3. Go to the Advanced tab. Give the x-direction scale factor the value 1.0 and the y-direction scale factor the value 20.0.
4. Click Remesh followed by OK.
5. Click the Solve menu and select Solver parameters.
6. Select the Stationary solver. Choose for Linear Solver the Direct (PARADISO) solver. Click OK.
7. Go to the Solve menu and select Solver manager.
8. Click the Solve For tab and select the Incompressible Navier-Stokes model.
    Now click the Solve button.
10. In the Times edit field type range(0,1,100), range(100,200,5000).
11. Go to the Time stepping tab and select for Method BDF. Click OK.
12. In the Solver Manager select the Convection-Diffusion model and click Solve.
Postprocessing

1. First a plot is made of the velocity field.
2. Go to the Postprocessing menu and click Plot Parameters.
3. Click the Surface tab.
4. From the Predefined quantities go to the Incompressible Navier-Stokes and select Velocity field.
5. Go to the Streamline tab and check the box Streamline plot. Again from the Predefined quantities select Velocity field.
6. Click Apply followed by OK.
7. Now make a plot of the concentration of soluble substrate, again go to Plot Parameters.
8. On the Surface tab go to the Predefined quantities, choose Convection-Diffusion and select Ss. Click Apply. A surface plot of Ss is made, showing the distribution of the concentration in the tank. The streamlines of the velocity are still displayed.
9. By following the steps above many (different type of) plots of the results can be made.
Bibliography


