

Internship MSc Systems and Control

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Abstract

This report analyses the performance, stability and robustness of the Witteveen en Bos (W+B) wastewater treatment controller called WOMBAT® (Witteveen+bos Optimal Model Based AeraTion). The controller modulates the oxygen set-point of the aerobic compartment in the Wastewater Treatment Plant (WWTP). The WWTP contains sludge (biomass); the bacteria in the sludge breaks down the environmentally hazardous ammonia, ammonium and nitrate nitrogen in the wastewater. Loosely speaking, a higher oxygen set-point prompts more oxygen to be supplied into the process, this in turn increases the rate in which the ammonia and ammonium are broken down by the bacteria in the aeration tank. We tested the performance, stability and robustness of the controller using the Benchmark Simulation Model (BSM).

Keywords: aeration, Activated Sludge Model (ASM), Benchmark Simulation Model (BSM), robustness, set-point, sludge, stability, Wastewater Treatment Plant (WWTP), WOMBAT®

Preface

As part of the curriculum of the Master System and Control at the University of Twente, every student is required to complete a 14 week (minimum) internship at a company or a scientific institute. My internship was from the beginning of January 2019 until the end of April 2019. The aim is to gain work experience at a company or institute at an academic level, i.e. carrying out research or delivering products or services to clients.

I did my internship at an engineering and consultancy firm, Witteveen en Bos (W+B). W+B specialises in offering consultancy services to the water, infrastructure, environment and building industries. Each area of expertise consists of so-called product-market combinations (PMCs). I did my internship in the PMC Digital Technologies department. The department consists of the following groups: process automation, data science and applications, geo-informatics, business development and asset management. I worked in the process automation group.

W+B was founded by architect W.G. Witteveen (1891-1979) and civil engineer G.S. Bos (1908-2004) in Deventer in 1946. The company consists of about 1100 employees (January 2019), seven offices in the The Netherlands and multiple international offices.

I sincerely appreciate the opportunity Witteveen en Bos gave me; to do my internship at their company in Deventer. The experience gave me invaluable insight into the inner workings of an engineering and consultancy firm. I would like to thank the entire PMC Digital Technologies department for their helpfulness and kindness, while I was carrying out my research at Witteveen en Bos. I would like to thank in particular my supervisor Erwin Visser for his guidance, wisdom and support!

Lastly, I would like to thank my Utwente supervisor, Gjerrit Meinsma, for his technical advice and for assessing my report.

Term dictionary

Acidification: a decrease in the pH

Aerobic: process requiring oxygen

Ammonification: a process where bacteria break down nitrogen-chemicals in waste into simpler chemicals, such as ammonia

Anaerobic: living or occurring in the absence of oxygen

Anoxic: an environment depleted of oxygen

Autotrophic: an organism capable of synthesizing its own food from inorganic substances

Eutrophication: an excessive amount of nutrients in a water body, leading to dense plant growth

Frequency response: the frequency spectrum in response to a stimulus signal

Heterotrophic: an organism that is unable to generate its own food and instead obtains food from plant or animal matter

Hydrolysis: the chemical breakdown of a compound due to a reaction with water

Influent: the wastewater entering the WasteWater Treatment Plant (WWTP)

Protozoa: microorganisms that feed on other microorganisms

Resonance frequency: a frequency exciting a resonance maximum in a system. These frequencies are often where the system could be unstable.

Run-off: rain water that enters the drains in urban areas and is often transported to the WWTP for treatment

Stoichiometry: the relationship between substances taking part in a reaction

Chapter 1: Introduction

1.1. Wastewater Treatment Plant (WWTP)

Wastewater treatment plants (WWTPs) are responsible for the cleansing of water from households, industrial processes and rain run-off that is supplied to the water plant through a series of pumps. In 2016 there was a reported total of 327 WWTPs in The Netherlands [1]. An overview of a typical WWTP is depicted in figure 1, taken from [3]. It can be observed that the process is split into 3 main phases: pre-treatment, biological treatment and post-treatment.

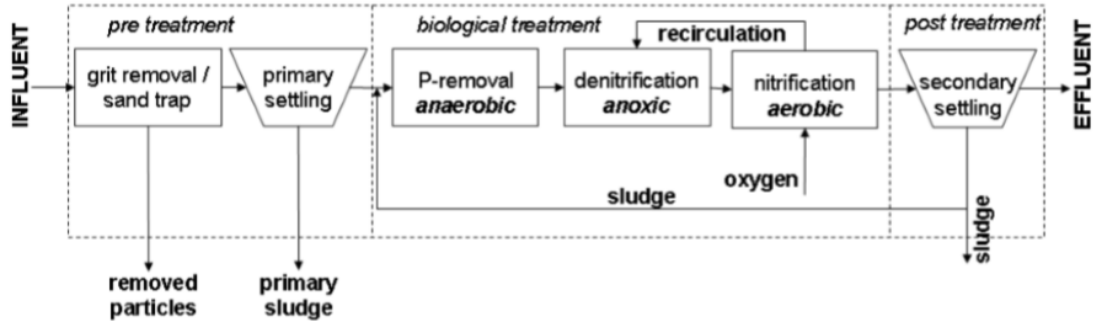


Figure 1: WWTP configuration overview. This image is taken from [3].

1.1.1. Influent

The influent depends on many factors. The most changeable variable in the influent is the flow rate, which is largely dictated by the weather conditions and daily/weekly human excretion and showering trends. The different weather conditions can be separated into the following categories: rain, dry and storm weather. During storm weather there are significant increases in the flow rate, due to intense periods of rain-fall. In contrast, the flow rate during rain weather is understandably greater than dry weather and typically lasts longer than storm rain-fall. On the other hand, the flow rate peaks are lower than that experienced during storm weather conditions. The influent is further influenced by the bathroom habits of the Dutch population. In the middle of the night there tends to be a low flow rate, because the majority of people are sleeping. Increased flow rate can be observed in the morning when people wake-up and in the late afternoon or early evening when people typically return home from work or school.

1.1.2. Pre-treatment

Initially, grit, sand and garbage (for instance plastic bottles or tree branches) are removed from the influent using grids. The resulting waste is compressed and transported to an external location for incineration.

Next, the water flows into the primary settling tank, where the water is stirred slowly. This causes the heavy particles to sink to the bottom of the tank, while the lighter particles rise to the surface. The heavy layer at the bottom is called the primary sludge and is removed from the process. The surface layer consisting mainly of grease and oil is skimmed off.

1.1.3. Biological treatment

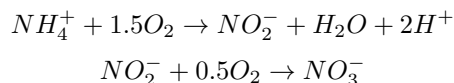
Nitrogen in wastewater can be discovered in the following forms: free ammonia (NH_3), ionized ammonia (NH_4^+), nitrate (NO_3^-), nitrite (NO_2^-) and as organic compounds. Summing the concentration of these nitrogen forms equals the total nitrogen content. Nitrogen is an essential nutrient for biological growth, but an excessive concentration of it should be avoided, since it can cause *eutrophication*. Eutrophication is the presence of excessive nutrients in a water body, leading to dense aquatic plant growth. This results often in

a layer of algae on the surface of the water body and subsequently deprives the aquatic organisms (e.g. fish) of oxygen. Furthermore, ammonia is toxic and excessive amounts can cause the death of aquatic organisms.

For the biological treatment of the water, a steady amount of sludge is kept in the process. This is achieved by removing excess waste sludge and recirculating the rest of the sludge. The sludge contains bacteria (*autotrophs* and *heterotrophs*) and *protozoa*. Heterotrophic bacteria survival depends on the consumption of another organism or organic carbon. Autotrophic bacteria are self-feeding organisms and are able to produce their own organic compounds [9]. This composition of bacteria facilitates the chemical reactions in the biological reactor (tank).

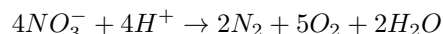
Water from the pre-treatment stage flows into the anaerobic section with the recirculated sludge. The biomass present in the anaerobic part contains micro organisms that break down organic material into readily biodegradable matter, emitting in the process biogas via *hydrolysis* and *acidification*. The biogas produced often consists of about 70% methane (CH_4) and 30% carbon dioxide (CO_2) with residual fractions of other gases (e.g. H_2 and H_2S). The bacteria consumes phosphate during this process. These processes occur in the absence of oxygen and nitrate.

Oxygen is present in the *aerobic* section of the reactor. The bacteria present convert ammonia (NH_4) into nitrate (NO_3). This reaction is known as *nitrification*. The nitrification reaction formula is:



The first step of the reaction represents the ammonia being oxidised to give nitrite. The second step represents the nitrite being oxidised to give nitrate. A greater concentration (below the saturation level) of dissolve oxygen (DO) speeds up the break-down of ammonia.

In the *anoxic* compartment, the DO concentration should be less than 0.5 mg/L. The nitrate produced in the aerobic section is broken down into nitrogen gas (N_2) within the anoxic section. The gas exits the tank via bubbles. This chemical reaction is called *denitrification* and is described by the following formula:



Note that the resulting oxygen is directly used to transform organic compounds into CO_2 and H_2O .

The water can go through the aerobic and anoxic section multiples times via recirculation to the anoxic section after the aerobic stage. This ensures that the nitrogen concentrations are low enough in the effluent.

1.1.4. Post-treatment

The biomass expelled from the biological treatment is removed from the liquid stream in the secondary settler. The sedimentation of the particles in the water is achieved by gravity combined with the density differences between the particles and water in the settler. A small portion of the sludge removed (consisting mainly of inert particles) and the rest (including active bacteria) is resupplied to the biological treatment phase.

1.1.5. Effluent

The effluent produced by the plant flows into the external water body, e.g. river, lake, ocean or wetlands.

1.2. Water quality requirements

To prevent potential harmful water entering the water bodies, the European Water Framework Directive water quality requirements need to be satisfied. In this paper we give more attention to the ammonia (plus ammonium) and total nitrogen threshold requirements, since these indicators show a stronger correlation

with the implementation of the WOMBAT® controller. It is more challenging to satisfy these requirements under stressed weather conditions, such as storm conditions. Typically during a storm the flow rate of the influent radically increases, thereby demanding more aeration in the aerobic compartment to keep the average ammonia below the upper-limits.

1.3. Benchmark Simulation Model (BSM)

The Benchmark Simulation Model (BSM) is used to carry out simulations on the WWTP in conjunction with the WOMBAT controller. The BSM provides a useful framework for control method comparison and is often used in wastewater treatment academia. Moreover, the framework defines a typical WWTP set-up, this includes for example the volume of the aeration and non-aeration compartments, *aerobic* and *anoxic* compartment dynamics and a typical WWTP influent.

1.4. Activated Sludge Model (ASM)

In order to effectively simulate a WWTP, the Activated Sludge Model (ASM) is used to simulate the reactions that take place in the anoxic and aerobic compartments in the biological reactor. Several ASM versions exist. We carried out our simulations with the most basic version ASM1, since this exhibits enough complexity for our purposes. Linearisation of this model reduces simulation times and allows you to more easily analyse the stability properties. The ASM is explained in greater detail in appendix B.

1.5. Stability

The stability of the WWTP is determined by analysing the impact of the influent on the effluent using the results of simulations. Further stability analysis is carried out in the frequency domain by linearising the ASM.

1.6. Aim of the report

This report seeks to answer the following questions:

1. Is the WOMBAT® able to control the nitrogen levels effectively under stressed conditions?
2. Is the WOMBAT® in conjunction with the WWTP (robustly) stable?

1.7. Report layout

The report is organised as follows:

- Chapter 2: BSM framework description and effluent quality indicators
- Chapter 3: A method of linearising the ASM1
- Chapter 4: Stability analysis of the ASM1 and the stability of a typical WWTP (with the WOMBAT® controller)
- Chapter 5: Simulation results from the linearised ASM1 and the BSM
- Chapter 6: Conclusions and recommendations

Chapter 2: Benchmark Simulation Model (BSM)

2.1. BSM introduction

"The Benchmark Simulation Model (BSM) is a detailed protocol for implementing, analysing and evaluating the impact and performance of both existing and novel control strategies applied to wastewater treatment plants (WWTPs)" (U.Jeppsson, 2008, pg.1).

IWA (International Water Association) Task Group and COST (European Cooperation in the field of Scientific and Technical Research) have produced two versions of the BSM. The first version is called BSM1. The BSM1 general overview can be found in figure 2. A description of the variables labeled is displayed in table 1. The second version, BSM2, was published in 2008. This version uses the BSM1 for the biological treatment of the wastewater and the sludge treatment. In addition, a primary clarifier, a thickener for the sludge wasted from the BSM1 clarifier, a digester for treatment of the solids wasted from the primary clarifier and the thickened secondary sludge have been added [11]. The BSM1 has three separate influent data files, simulating the following weather events: rain, dry and storm. These datasets contain influent data for 14 days, whereas the BSM2 has one dynamic dataset containing 609 days of a mixture of storm, rain and dry weather conditions.

For the analysis of the whole WWTP we used primarily the BSM2, because despite higher computation times it simulates a WWTP closer than the BSM1 version.

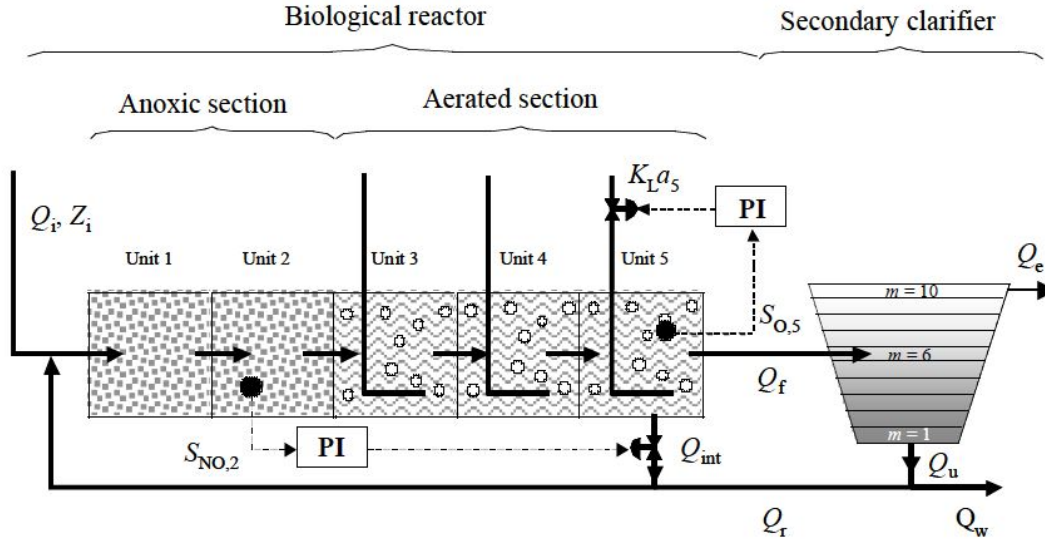


Figure 2: BSM1 general overview. This image is taken from [10].

Variable	Description
Q_i	Influent flow rate [m ³ /d]
Q_f	Flow rate between unit 5 and the secondary clarifier [m ³ /d]
Q_e	Effluent flow rate [m ³ /d]
Q_{int}	Internal recycle flow rate from compartment 5 [m ³ /d]
Q_r	External recycle flow rate from the underflow of the secondary clarifier [m ³ /d]
Q_w	Wastage flow rate [m ³ /d]
Q_u	Underflow rate of the secondary clarifier [m ³ /d]
Z_i	Influent concentration
$S_{NO,2}$	Nitrate concentration in unit 2
$S_{O,5}$	Dissolved oxygen concentration in unit 5
K_{La5}	Oxygen transfer coefficient applied to unit 5 [d ⁻¹]

Table 1: Description of variables in figure 2.

2.2. BSM features of interest

The BSM models use the ASM1 (Activated Sludge Model no. 1) model to accurately simulate the biological treatment section of the process. More information about the ASM1 can be found in appendix B.

As can be observed in figure 2, the bioreactor is made up of 5 compartments: 2 non-aerated compartments (units 1 and 2) and 3 aerated compartments (units 3 to 5). For the BSM2, each non-aerated compartment has a volume of 1,500 m³ and aerated compartment a volume of 3,000 m³.

The two PI (Proportional Integral) controllers are implemented for control of aeration compartment and control of recirculation of wastewater back to the non-aerated compartments. The PI controller for control of the aeration compartment using measurements from compartment 5, determines the oxygen transfer coefficient K_{La5} of the aeration equipment under the operating conditions imposed [2]. The coefficient depends on temperature and is calculated using the following formula

$$K_{La}(T) = 1.024^{T-15} \cdot K_{La}(15^\circ\text{C})$$

where T denotes temperature in degrees and $K_{La}(15^\circ\text{C})$ is the transfer coefficient at 15°C.

The oxygen saturation point is also modelled in the BSM2 and is dependent on temperature. A decrease in the temperature leads to a decrease in the saturation point.

$$S_{O,as}^{\text{sat}} = 0.9997743214 \cdot \frac{8}{10.5} \cdot 6791.5 \cdot K(T_K)$$

where $K(T_K) = 56.12e^{A+B/T^*+C\ln T^*}$, $T^* = T_K/100$ (K), $T_K = T_{as}(^\circ\text{C})+273.15$, $A = -66.7354$, $B = 87.4755$ and $C = 24.4526$. The formula is valid in the range 273.15 K - 348.15 K (Kelvin) [11].

The effluent S_{NH} (ammonia and ammonium) limit is 4 g N.m⁻³ for BSM, as opposed to 2 g N.m⁻³ imposed by the European Water Framework Directive 2000. The latter is taken as the quality limit in this report, since W+B adheres to the European Water Framework Directive 2000. Furthermore, the framework requires that the total nitrogen (sum of nitrate, nitrite, ammonia and ammonium) is below 10 g N.m⁻³. Instead, the BSM nitrogen limit takes into account the organic nitrogen.

2.3. BSM performance indicators

The **Aeration Energy (AE)** [kWh.d⁻¹] takes into account the plant peculiarities (type of diffuser, bubble size, depth of submersion, etc.) and is calculated using the oxygen transfer coefficient K_{La} [1/d]

according to the following relation

$$AE = \frac{1}{t_{obs} \cdot 1.8 \cdot 1000} \int_{t=245days}^{t=609days} \sum_{k=1}^5 V_{as,k} \cdot K_L a_k(t) dt$$

where k refers to the compartment number [11].

The total Kjeldahl nitrogen is the sum of organic nitrogen, ammonia (NH_3), and ammonium (NH_4^+). The Kjeldahl nitrogen is calculated as follows

$$S_{NKj,e} = S_{NH,e} + S_{ND,e} + X_{ND,e} + i_{XB}(X_{B,H,e} + X_{X,A,e}) + i_{XP}(X_{P,e} + X_{i,e})$$

The letter e in the subscripts symbolises effluent. The coefficients i_{XP} and i_{XB} are *stoichiometric* parameters taken from the ASM. A description of the parameters and a description of the concentrations can be found in appendix B in table 8 and table 5 respectively.

The effluent quality can be measured using the **Effluent Quality Index (EQI)** [kg pollution unit.d⁻¹]. Ensuring good effluent quality prevents levies and fines for the discharge of polluted water in the receiving water bodies. The EQI is averaged over the period of observation t_{obs} (365 days \approx 1 year) based on a weighting of the effluent loads of compounds that have a significant impact on the quality of the receiving water and that are usually included in regional legislation [11]. The relevant formula is:

$$EQI = \frac{1}{t_{obs} \cdot 1000} \int_{t=245days}^{t=609days} \left(B_{TSS} \cdot TSS_e(t) + B_{COD_e}(t) \cdot COD_e(t) + B_{NKj} \cdot S_{NKj,e}(t) \right. \\ \left. + B_{NO} \cdot S_{NO,e}(t) + B_{BOD5} \cdot BOD_e(t) \right) Q_e(t) \cdot dt \quad (1)$$

where TSS (Total Suspended Solids) denotes the solids in the water that can be trapped by a filter, COD (Chemical Oxygen Demand) is the amount of oxygen that can be used in the biological tank reactions, NKj the Kjeldahl nitrogen, NO the nitrate and BOD (Biochemical Oxygen Demand) is the amount of oxygen used by the biomass in the biochemical reactions.

The BSM is a useful standard that is often used in the academic world to theoretically test control methods. This allows for effective comparison of control techniques. In the coming chapters the BSM is used to test the WOMBAT and the PI controller that is used to compute the oxygen set-point for aeration in the aerobic compartments. We are going to compare the following indicators: total nitrogen ($S_{NH} + S_{NO}$), Kjeldahl nitrogen, ammonia (and ammonium) S_{NH} , nitrate S_{NO} , AE and EQI.

Chapter 3: Activated Sludge Model no. 1 (ASM1)

linearisation and stability analysis

3.1. ASM1 linearisation set-up

The activated sludge model no. 1 (ASM1) models the reactions that occur in the *aerobic* and *anoxic* compartments in the biological reactor. The model consists of 13 differential equations and can be represented with the following formula

$$\frac{dz_j}{dt} = \sum_{i=1}^8 \nu_{i,j} \rho_i(t), \quad 1 \leq j \leq 13, \quad (2)$$

where z_j denotes the concentration, $\nu_{i,j}$ the *stoichiometric* coefficient and ρ_i the process rate. Information on how to derive these formulas and concentrations can be found in appendix B.

The reaction rates within the ASM1 contain so-called continuous 'switch functions' and are able to switch 'on' or 'off' depending on the conditions in the biological reactor [2]. Consider as an example the following switch function

$$\frac{S_O}{K_{O,H} + S_O}$$

where S_O is the concentration of dissolved oxygen (DO) and $K_{O,H}$ is the oxygen half-saturation coefficient for *heterotrophic* bacteria. This particular switch function is present in the reaction rate responsible for the aerobic growth of heterotrophs:

$$\rho_1 = \hat{\mu}_H \cdot \frac{S_S}{K_S + S_S} \cdot \frac{S_O}{K_{O,H} + S_O} \cdot X_{B,H} \quad (3)$$

where $\hat{\mu}_H$ is the heterotrophic maximum specific growth rate, S_S is the concentration of readily biodegradable substrate, $X_{B,H}$ the active heterotrophic biomass and K_S the half-saturation coefficient for heterotrophs. It can be observed that the reaction rate tends to zero as S_O tends to zero. Thus, an absence of oxygen switches the term 'off'. Conversely, non-zero values switches the term 'on'. The value of $K_{O,H}$ is for our simulations set equal to 0.2 [g O₂ m⁻³]. It can be verified that the function is continuous (assuming positive values of S_O). Continuity is needed to simulate without encountering infinite values.

Equation 2 is expanded, so that it is possible to incorporate inputs into the compartment. The expansion is represented as follows

$$\frac{dz_j}{dt} = \sum_{i=1}^8 \nu_{i,j} \rho_i(t) + \frac{Q(t)}{V} (z_{in,j}(t) - z_j(t)), \quad 1 \leq j \leq 13, \quad (4)$$

where $z_{in,j}(t)$ denotes the influent concentration into the compartment, $Q(t)$ the influent flow rate, V the compartment volume and $\frac{Q(t)}{V}$ the dilution rate [8].

The ASM1 is restrictive, due to its simplicity. For instance it assumes that the temperature is constant, i.e. the coefficients are derived beforehand based on temperature. Furthermore, the model assumes that the pH is constant and near neutrality [2]. Although, it is deemed sophisticated enough to carry out our simulations with sufficient accuracy for stability analysis purposes.

The concentration steady states provided by the Benchmark Simulation Model (BSM) [10] are taken as the linearisation point. The steady states are generated using a 100-day period of stabilisation in the closed-loop system (with feedback control) using constant inputs.

3.2. ASM1 anoxic compartment linearisation

Consider a continuous-time system described by the *nth-order* state-space model

$$\frac{d\mathbf{z}}{dt} = \mathbf{A}\mathbf{z} + \mathbf{B}\mathbf{u} \quad (5)$$

$$\mathbf{y} = \mathbf{C}\mathbf{z} + \mathbf{D}\mathbf{u} \quad (6)$$

where \mathbf{z} denotes the state vector, \mathbf{u} the input vector and \mathbf{y} the output vector. The matrix \mathbf{A} has dimension $n \times n$, \mathbf{B} dimension $n \times m$, \mathbf{C} dimension $p \times n$ and \mathbf{D} dimension $p \times m$, where n , m and p are natural numbers ($\mathbb{N} = 1, 2, 3, \dots$). The *order* of the system is equivalent to the number of states in the state vector \mathbf{z} .

The state (13 ASM1 concentrations) and input are chosen for the linearisation as follows

$$\begin{aligned} \mathbf{z}(t) &= [S_I, S_S, X_I, X_S, X_{BA}, X_{BH}, X_P, S_O, S_{NO}, S_{NH}, S_{ND}, X_{ND}, S_{ALK}]^T \\ \mathbf{u}(t) &= [S_{I,in}, S_{S,in}, X_{I,in}, X_{S,in}, X_{BA,in}, X_{BH,in}, X_{P,in}, S_{O,in}, S_{NO,in}, S_{NH,in}, S_{ND,in}, X_{ND,in}, S_{ALK,in}]^T \end{aligned}$$

where once again 'in' symbolises influent in the subscript. More information about the state variables can be found in the appendix B. The rate expressions ρ_i are modelled in a linear form respective to their variables [8]. For instance in non-linear form ρ_1 is as seen in equation 3 and in the suggested linear form:

$$\rho_1 = a_{1,2}S_S + a_{1,5}X_{BH} + a_{1,8}S_O$$

where the parameters $a_{1,2}$, $a_{1,5}$ and $a_{1,8}$ are to be estimated. The first index of the parameters stands for the reaction rate number and the second for the rank of the corresponding variable in the state space vector \mathbf{z} . The rates ρ_4 and ρ_5 are already linear, but are transformed to the same coefficient notation: $\rho_4 = a_{4,5}X_{BH}$ and $\rho_5 = a_{5,6}X_{BA}$. The linear reaction rate vector is put into the following form

$$\rho = [\rho_1, \rho_2, \rho_3, \rho_4, \rho_5, \rho_6, \rho_7, \rho_8]^T$$

The parameters $a_{4,5}$ and $a_{5,6}$ are not estimated because they are equal to the stoichiometric parameters b_H and b_A respectively.

Taking the flow rate $Q(t)$ to be constant over time, allows you to form a LTI (Linear Time-Invariant) state-space model with the following matrices

$$\mathbf{A} = \mathbf{W}\Phi - \frac{\tilde{\mathbf{Q}}}{\bar{V}}, \quad \mathbf{B} = \frac{\tilde{\mathbf{Q}}}{\bar{V}}\mathbf{I}, \quad \mathbf{C} = \mathbf{I}, \quad \mathbf{D} = \mathbf{0} \quad (7)$$

where \mathbf{W} is the so-called stoichiometry matrix, i.e. containing the stoichiometry coefficients (more information in appendix B). Φ is the matrix of parameters that needs to be estimated. The dimensions of \mathbf{W} and Φ are 13×8 and 8×13 respectively. \mathbf{I} is the 13×13 identity matrix. $\tilde{\mathbf{Q}}$ denotes the average influent rate.

3.3. ASM1 aerobic compartment linearisation

For the aerobic compartment, the S_O concentration mass balance equation (in the ASM1) is extended to incorporate the effect of external air flow. The additional term is $k_L a (S_O^* - S_O)$ where S_O^* is the oxygen concentration at saturation. The factor $k_L a$ represents the transfer coefficient of the external aeration system. The oxygen saturation S_O^* is dependent on the temperature and is incorporated into the aerobic state-space model by extending the input vector so that

$$\mathbf{u}(t) = [S_{I,in}, S_{S,in}, X_{I,in}, X_{S,in}, X_{BA,in}, X_{BH,in}, X_{P,in}, S_{O,in}, S_{NO,in}, S_{NH,in}, S_{ND,in}, X_{ND,in}, S_{ALK,in}, S_O^*]^T$$

This leads to the following state-space definition

$$\mathbf{A} = \mathbf{W}\Phi - \left(\frac{\tilde{\mathbf{Q}}}{\bar{V}} + \text{Diag}(\mathbf{J}) \right), \quad \mathbf{B} = \left(\frac{\tilde{\mathbf{Q}}}{\bar{V}} \mathbf{I} | \mathbf{J} \right), \quad \mathbf{C} = \mathbf{I}, \quad \mathbf{D} = \mathbf{0} \quad (8)$$

where

$$\mathbf{J} = [0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ k_L a \ 0 \ 0 \ 0 \ 0]^T$$

\mathbf{B} has been modified in accordance with \mathbf{u} and has dimension 13×14 . \mathbf{A} has been modified in order to take into account the term $k_L a \cdot S_O$ in the S_O mass balance equation. $\text{Diag}(\mathbf{J})$ is the diagonal matrix with \mathbf{J} as the diagonal entries. The dimensions of \mathbf{C} and \mathbf{A} remain unchanged and matrix \mathbf{D} now has dimension 13×14 [8].

3.4. Identification procedure

The parameters for ρ_i for $i = 1, 2, 3, 6, 7, 8$ can be derived using the least squares algorithm [8]. The linearised forms for ρ_i can be seen in appendix C. We denote the vector of parameters by θ_i and the given states involved in the linear equation as M_i . Consequently, the linear models can be described in vector form as $\rho_i = M_i \theta_i$ for $i = 1, 2, 3, 6, 7, 8$. For example, ρ_1 consists of $M_1 = [S_S \ X_{BH} \ S_O]$ and $\theta_1 = [a_{1,2} \ a_{1,5} \ a_{1,8}]^T$. The parameter vectors θ_i are estimated by minimising the quadratic cost functions $F_i = (\rho_{i,ASM1} - M_i \theta_i)^2$ by using the least square algorithm. $\rho_{i,ASM1}$ denotes ρ_i calculated directly from the non-linear ASM1 model. We use the steady state values to compute $\rho_{i,ASM1}$.

The estimated parameters are set (based on their second index) in vectors $\hat{\Phi}_i$ for $i = 1, 2, 3, 6, 7, 8$. If there does not exist a parameter for a given entry in the vector, the entry is equal to zero. The already known parameters from ρ_4 and ρ_5 are also placed into vectors $\hat{\Phi}_4 = \Phi_4$ and $\hat{\Phi}_5 = \Phi_5$. The vectors are then concatenated to form

$$\hat{\Phi} = [\hat{\Phi}_1 \ \hat{\Phi}_2 \ \hat{\Phi}_3 \ \hat{\Phi}_4 \ \hat{\Phi}_5 \ \hat{\Phi}_6 \ \hat{\Phi}_7 \ \hat{\Phi}_8]$$

The computed $\hat{\Phi}$ is substituted into equations 7 and 8 to calculate the state-space for the anoxic and aerobic compartments.

3.5. Pros and cons of linearising the ASM1

Pros:

- The linearised ASM1 gives rise to shorter simulation times, since the non-linear ASM1 is stiffer, i.e. smaller steps needed for satisfactory results, due to strong variations in nearby solutions.
- Casting the model into a state-space form allows you to more easily see the relationship between the inputs and outputs. Bode plots and step responses can also be executed to give more insight into the relationships.
- It is easier to determine if the system is stable, i.e. pole derivation (more information can be found in chapter 4).

Cons:

- The linearised version does not model the biological reactor as closely as the original ASM1, since the complexity of the non-linear reaction rates is removed.
- The linearisation point is subject to change, because realistically there does not exist a steady state in a Wastewater Treatment Plant (WWTP).
- Linearising removes the ASM1 switch functions, leading to possible concentration values below zero. From the point a concentration is recorded as a negative value, the simulation is void, since a negative value of one concentration has a knock-on effect on the calculations of the other mass balance equations.
- To derive a LTI system, the dilution rate is taken as a constant, whereas in a actual WWTP the influent flow is varying with time.

Chapter 4: Stability analysis

4.1. Pole stability analysis

The poles of the continuous system are the eigenvalues of the state-space matrix \mathbf{A} (as seen in equation 5 in chapter 3) [4]. The stability of the system is subsequently analysed by observing where the poles lie on the complex plane. Stability is verified if the plotted poles lie on the left hand plane, i.e. the real part is less than zero.

4.2. BIBO (Bounded-Input/Bounded-Output) stability

Our system is a closed-loop system and the block diagram representation can be viewed in figure 3. The symbol \mathbf{y} is the output signal, \mathbf{e} the error signal, \mathbf{r} the reference signal and \mathbf{u} the input signal. The subscript O2 stands for oxygen and NH for ammonia (and ammonium). The model contains two controllers: the WOMBAT® controller and a PI (proportional integral) controller. The WOMBAT® controller supplies the oxygen set-point and is subtracted by the dissolved oxygen (DO) measurement (S_O) in the reactor, giving the oxygen error (e_{O2}). Feeding the error as the input into the PI controller produces u_{O2} . The input into the plant (u_{O2}) is the oxygen transfer coefficient $k_L a$ and is used by the aeration equipment to aerate the aerobic compartments.

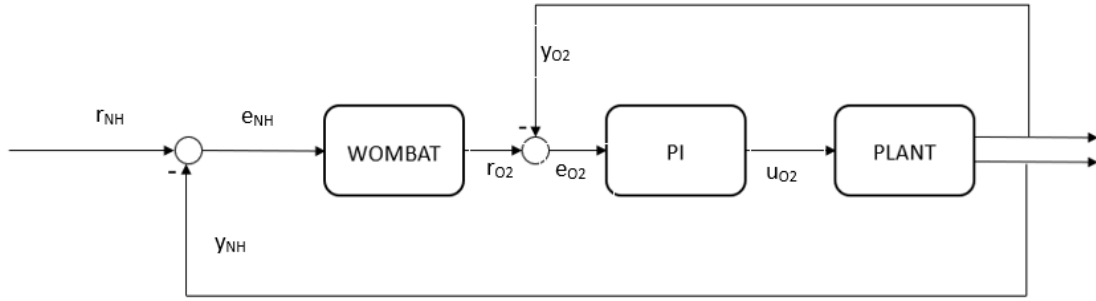


Figure 3: Block diagram of a closed-loop system. This set-up is used by Benchmark Simulation Model (BSM). Note that $u_{O2} = r_{O2}$.

The control system is considered BIBO *stable* if every bounded input signal \mathbf{r} results in bounded output signals \mathbf{e} , \mathbf{u} and \mathbf{y} [5]. Moreover, a signal is considered bounded if it has finite values.

4.3. Robust stability

It was not possible to determine if the system is robustly stable using the Additive Uncertainty Model (and the Multiplicative Uncertainty Model) as depicted in figure 4, since the *actual* plant \tilde{P} needs to be derived. In other words, \tilde{P} is used in the calculation of the perturbation ($W_A \Delta_A$), where W_A is a stable filter modeling the additive uncertainty ($\tilde{P} - P$) and Δ_A is a perturbation with maximum unity infinity norm ($\|\Delta_A\|_\infty \leq 1$). The nominal plant P is a simplification of the actual plant and can be derived using the Activated Sludge Model (ASM).

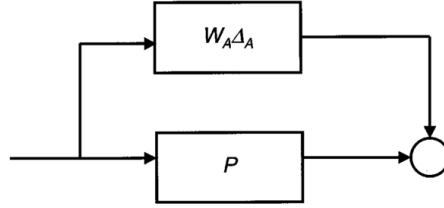


Figure 4: Additive Uncertainty Model. P denotes the nominal plant. Taken from [12].

The actual plant of many systems is often derived by manually sweeping over a frequency range of interest (usually around the *resonance frequencies* of the system) using a signal generator. This produces a *frequency response*, which can be used to estimate the actual transfer function. This technique may be possible to apply on a Wastewater Treatment Plant (WWTP).

Chapter 5: Simulation results

5.1. Linearised aerobic compartment

Figure 5 shows the concentration of ammonia (and ammonium) and nitrate over 7 days in a aerobic compartment at temperatures 15° and 5°. The simulation is carried out using the linearised state-space Activated Sludge Model no. 1 (ASM1) that is derived using the theory from chapter 3. The simulation uses the BSM1 *rain influent* and interpolation of the influent dataset is applied to give a more detailed plot. We interpolated between data points p_i and p_{i+1} , using the following formula:

$$p_{int,j} = \frac{j}{n}(p_{i+1} - p_i) + p_i$$

where $p_{int,j}$ is the interpolated data point j between the two data points. The index i denotes the original data set entry and n is the total data points interpolated plus one. The purpose of the plot is to demonstrate the impact of the temperature on the biological reactions in the aerobic compartment.

To allow control of the dissolved oxygen (DO) level in the compartment, the ASM1 oxygen S_O balance equation was removed and the DO is used only as an input [13]. This input is taken as a constant oxygen set-point and set equal to 2 g (-COD)/m³.

The stability of the oxygen set-point controlled state-space ASM1 is verified by plotting the poles (see appendix C) and observing that they lie on the left hand plane on the complex plane. This is to be expected, since in Wastewater Treatment Plants (WWTPs) unstable behaviour does not occur. In real life concentrations are finite, therefore WWTPs are always BIBO stable.

At a higher temperature in the aerobic compartment the ammonia (and ammonium) S_{NH} is considerably lower, due largely to greater aerobic growth of heterotrophic bacteria ρ_1 and autotrophic bacteria ρ_3 (see table 2). Thereby increasing the rate of S_{NH} breakdown via the nitrification reaction. Leading to an increase in the nitrate concentration S_{NO} . The daily peaks and troughs can be explained by the human bathroom habits, i.e. a greater bathroom usage by the population causes higher S_{NO} and S_{NH} load in the WWTP influent. The results of the other component simulations and the implementation in MATLAB® can be viewed in appendix C.

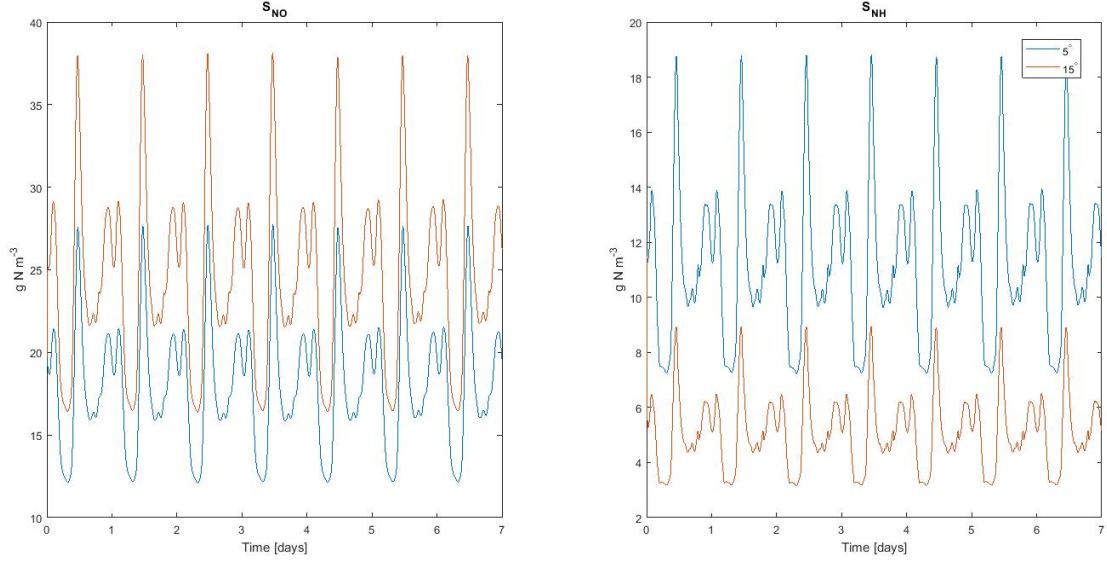


Figure 5: S_{NO} (nitrate and nitrite) and S_{NH} (ammonium and ammonia) concentration in the aeration compartment plot.

Reaction rate [1/d]	5°	15°
Aerobic growth of heterotrophs (ρ_1)	391.9081	696.7255
Anoxic growth of heterotrophs (ρ_2)	30.2349	53.7508
Aerobic growth of autotrophs (ρ_3)	10.1383	28.162
Decay of heterotrophs (ρ_4)	341.7135	768.8554
Decay of autotrophs (ρ_5)	2.7749	7.7082
Ammonification of soluble organic nitrogen (ρ_6)	54.4965	85.1507
Hydrolysis of entrapped organics (ρ_7)	773.2597	1113.5
Hydrolysis of entrapped organic nitrogen (ρ_8)	56.6784	81.6169

Table 2: Comparison of the reaction rates [1/d] for temperatures 5° and 15°.

5.2. Benchmark Simulation Model 2 (BSM2)

The BSM2 incorporates temperature. Changes in the temperature results in a change in the coefficients in the Activated Sludge Model, thereby affecting the biological reaction speeds. Figure 6 shows a plot of the modelled temperature over 609 days. It can be noted that the plot has a sinusoidal form with added noise, giving a large temperature variation.

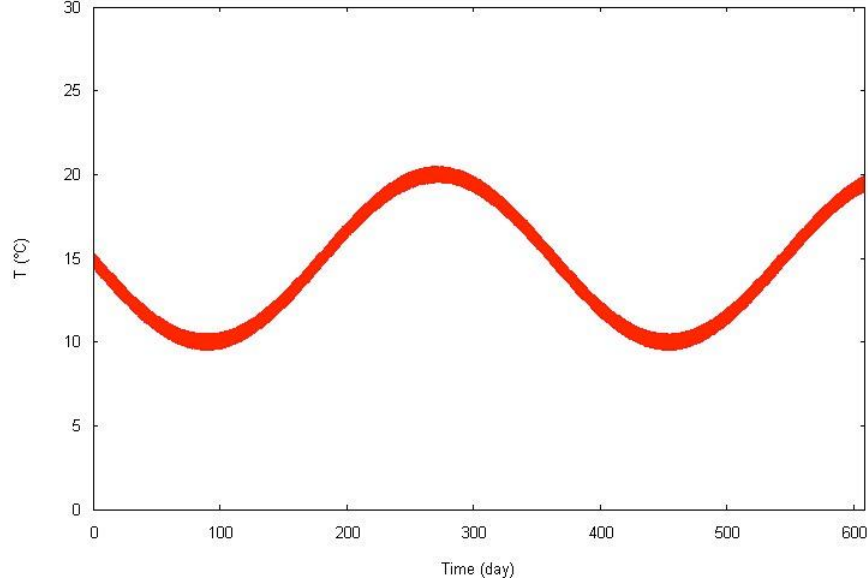


Figure 6: BSM2 temperature plot.

For quicker and more insightful simulations, a 100 days (245 to 345) from the BSM2 609 day influent dataset was extracted containing a mixture of storm, rain and dry weather conditions. The range of weather conditions enabled us to carry out effective system stress testing on the WOMBAT and PI controller. In particular, the influent flow ranges from 5,146 to 85,841 [m³/d].

Figure 7 implies that the ammonia concentration S_{NH} is comfortably under the upper-limit set by the European Water Framework Directive 2000 for the majority of the simulation. More specifically, the effluent ammonia nitrogen upper-limit (2 g N/m³) was violated during approximately 1.2 days and the average for the whole simulation was around 0.53. The peaks in ammonia can be partly explained by the storm or wet weather conditions, that lead to a spike in the influent flow.

Looking at figure 9, its clear that the total nitrogen level (S_{NH} and S_{NO}) remains mostly under the limit (10 g N/m³). The upper-limit was violated during 17.3 days. Therefore, the WOMBAT® performs reasonably.

In figure 12, the EQI increases when the nitrogen levels rise, since the EQI equation 1 is based heavily on the nitrogen concentrations.

Comparing figure 11 with the nitrogen plots, it can be noted that the aeration energy [kWh/d] increases when there is an increase in the ammonia level. This is due to an increase in the oxygen set-point from the WOMBAT® controller in accordance with the elevated ammonia levels.

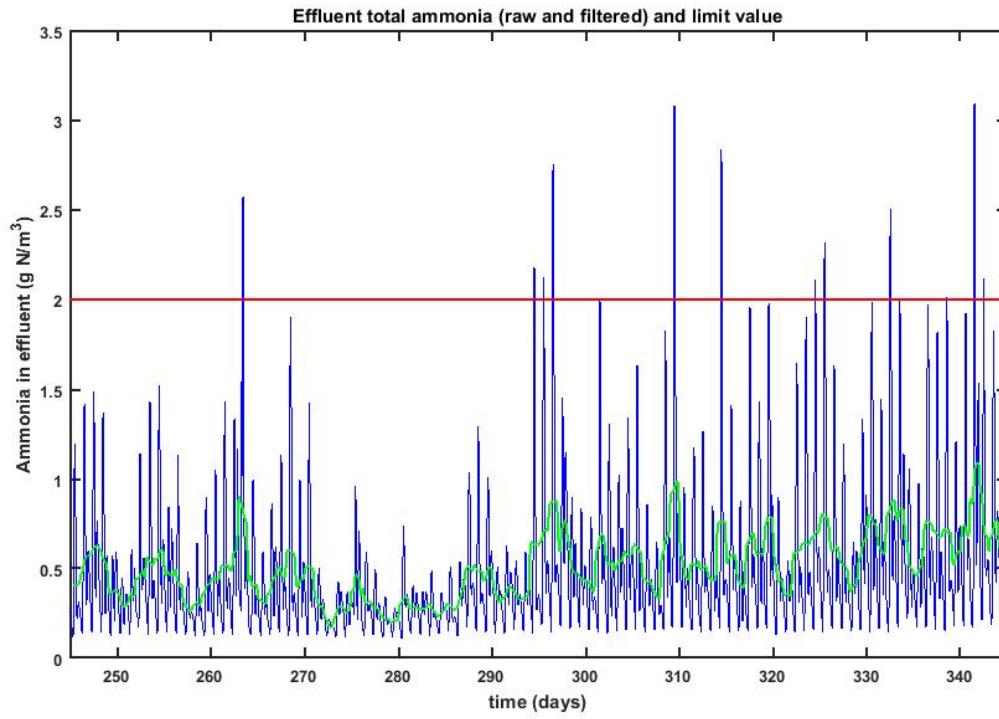


Figure 7: WOMBAT® S_{NH} control

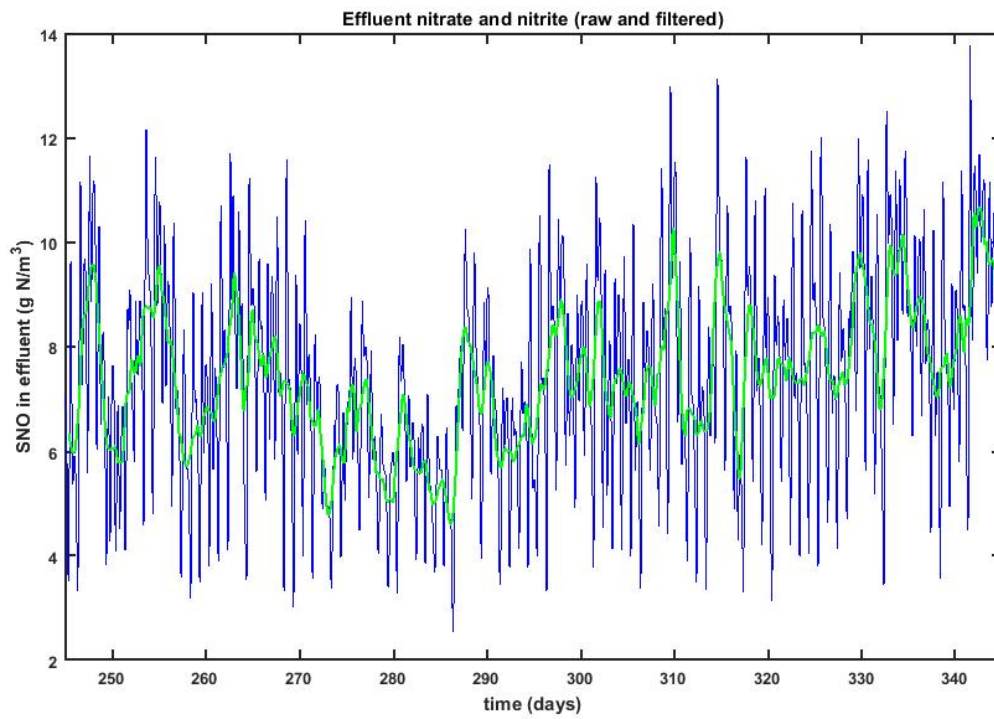


Figure 8: WOMBAT® S_{NO} control

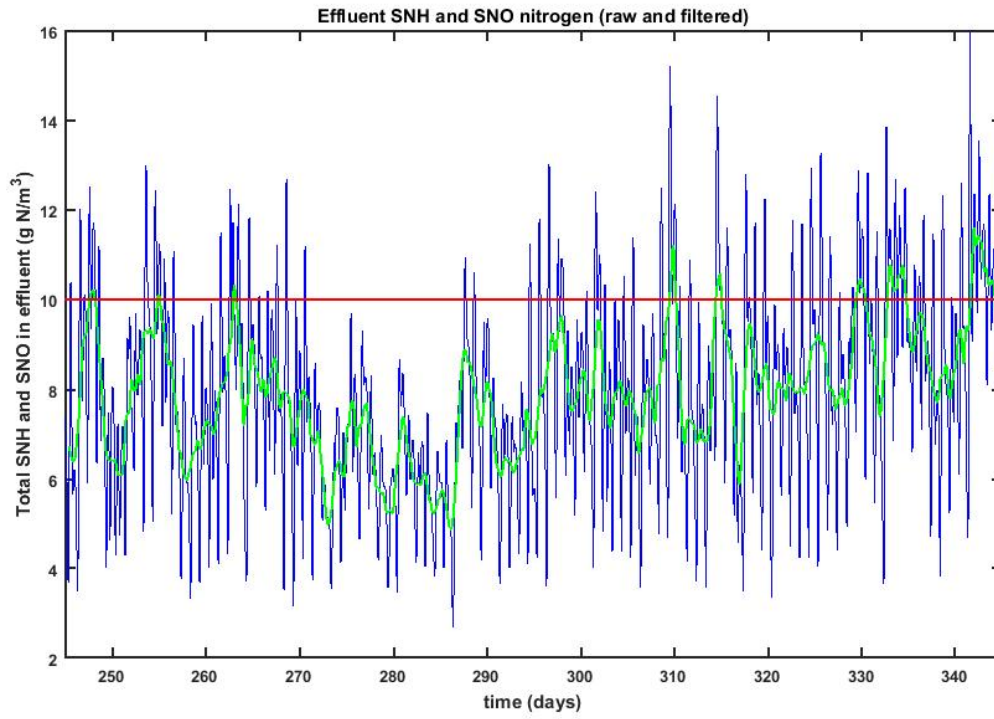


Figure 9: WOMBAT® S_{NO} and S_{NH} control

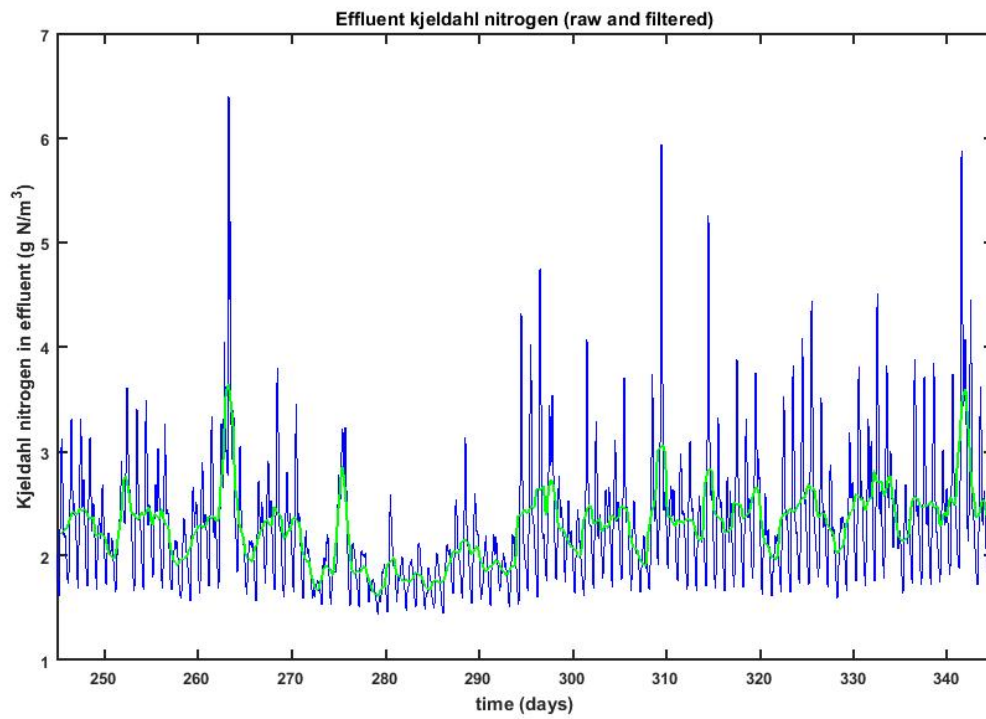


Figure 10: Kjeldahl effluent. The WOMBAT® is used for this simulation.

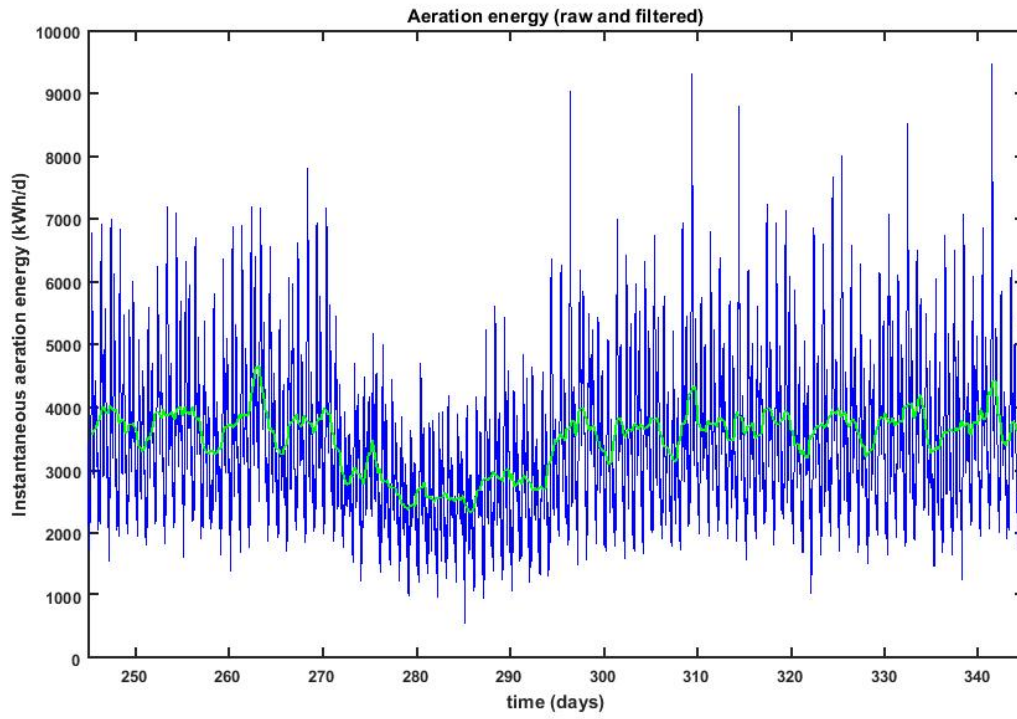


Figure 11: Aeration energy. The WOMBAT® is used for this simulation.

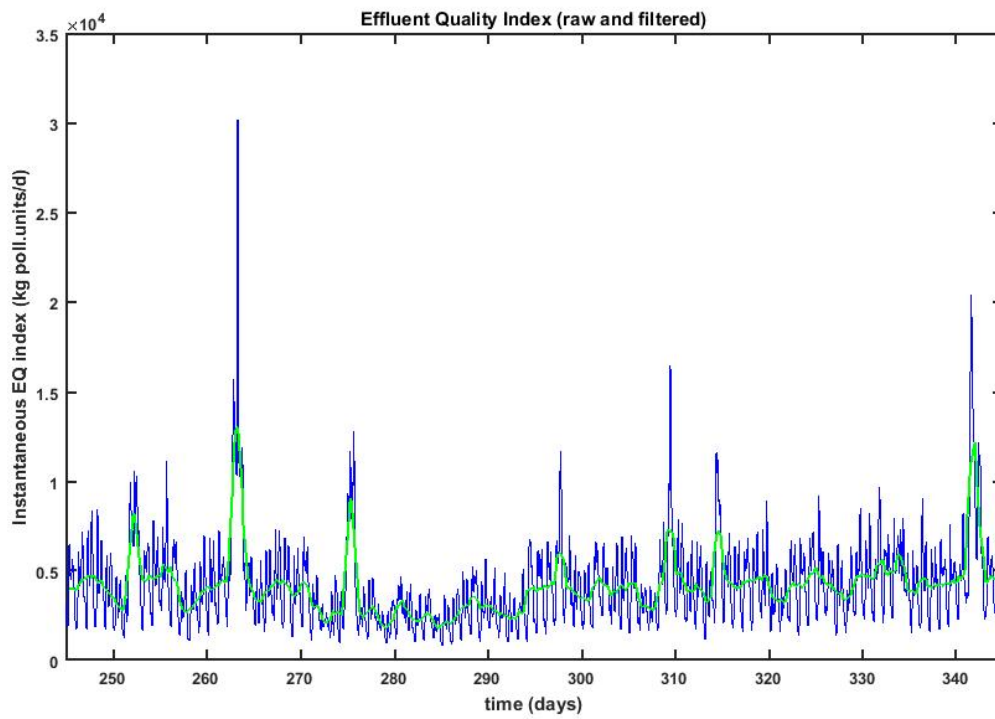


Figure 12: EQI. The WOMBAT® is used for this simulation.

5.3. The WOMBAT® controller versus a typical PI controller

A PI (Proportional Integral) controller was implemented using typical gain values (taken from WWTP PI controllers) and has the following form:

$$O_{2,set} = (P + I \frac{1}{s}) \cdot e(t)$$

where P is the proportional gain, I the integral gain, $\frac{1}{s}$ represents the mathematical integration operation, $e(t)$ is the error dependent on time and $O_{2,set}$ the oxygen set-point. The error is generated by taking the difference of the ammonia (and ammonium) S_{NH} measurement and the S_{NH} set-point (see figure 3). Note that the set-point for the ammonia is set to 1.5 g N/m³.

In table 3 it can be seen that although the WOMBAT® performs marginally better for the average total nitrogen concentration ($S_{NH} + S_{NO}$), there is not a substantial difference between the performance of the two controllers. This could be due to the BSM2 set-up, where ammonia (and ammonium) concentrations in the compartments are relatively low when the oxygen set-point is constantly 0.5 mg/L.

In the BSM1 set-up, there is generally a higher concentration of ammonia (and ammonium) in the compartments. The better performance of the WOMBAT® controller can be clearly identified in the results from the BSM1 simulations. The effluent indicators are compared for the two controllers in table 4. Notice that the total nitrogen is lower when the WOMBAT® controller was used. This is due to the predictive nature of the controller, where it is designed to forecast the optimal oxygen set-point, i.e. predicts the oxygen set-point that gives the lowest total nitrogen level at any given point in time. Alternatively, the PI controller attempts to maintain the S_{NH} at set-point 1.5 g N/m³, using the error between the set-point and the actual measurement in the aerobic compartment regardless of the effect of converting the ammonia (and ammonium) to nitrate (nitrification). Consequently, the control with the WOMBAT® results in higher ammonia levels, but more importantly a lower total nitrogen level. Note that, it is possible to adjust the proportion of the ammonia converted to nitrate, by updating the value of a certain parameter in the WOMBAT® control algorithm.

The aeration energy is higher for the PI controller, since it used more aeration to lower the ammonia via the nitrification reaction. Both controllers do not satisfy the effluent quality upper-limits in the BSM1 results. This could be due to a variety of reasons concerning the set-up of the BSM1. For instance the lack of a primary clarifier in the process, thereby excluding the pre-processing of the influent and recirculated sludge or the capacity of the compartments in the biological reactor are too small for dealing with the ammonia and nitrate load. Each BSM1 aerobic compartment has volume 1333m³ and each anoxic compartment 1000m³.

Indicator averages	PI controller	WOMBAT® controller
Ammonia (and ammonium) S_{NH} [g N/m ³]	0.52	0.53
Nitrate (and nitrite) S_{NO} [g N/m ³]	7.44	7.42
S_{NH} and S_{NO} [g N/m ³]	7.97	7.95
Kjeldahl nitrogen [g N/m ³]	2.40	2.42
Aeration Energy (AE) [kWh/d]	3495.43	3491.80
Effluent Quality Index (EQI) [kg poll.units/d]	4188.40	4191.22

Table 3: Comparison of the PI and WOMBAT® effluent quality indicators using the BSM2.

Indicator averages	PI controller	WOMBAT® controller
Ammonia (and ammonium) S_{NH} [g N/m ³]	2.02	3.50
Nitrate (and nitrite) S_{NO} [g N/m ³]	14.08	10.43
S_{NH} and S_{NO} [g N/m ³]	16.10	13.93
Kjeldahl nitrogen [g N/m ³]	3.96	5.48
Aeration Energy (AE) [kWh/d]	5022.24	3433.90

Table 4: Comparison of the PI and WOMBAT® effluent quality indicators using the BSM1 (dry weather influent).

The system is proved to be **BIBO stable**, since the simulations were completed with bounded-outputs resulting from the bounded-input values.

Chapter 6: Conclusions and recommendations

6.1. Conclusions

The Benchmark Simulation Model (BSM) is used for testing the stability of the WOMBAT® controller, since it is widely recognised in academia. Moreover, BSM defines the dynamics of a typical Wastewater Treatment Plant (WWTP) and provides effluent quality indicators, which enables effective comparison of control methods. The newest version (BSM2) provides a more sophisticated model of the WWTP. Although, the complexity of BSM2 causes large simulation times. In real life WWTPs vary in their set-up. Therefore, the BSM set-up may not suitably simulate certain WWTPs. Furthermore, the mathematical models used in the BSM do not completely mimic the complexity of real life WWTPs. For instance, the adding of chemicals to neutralise the pH in the WWTP is not taken into account. In fact, some WWTPs treat wastewater solely with chemicals. In such a WWTP, a controller to determine the oxygen set-point is redundant, since no aeration is required. Thus, it is advised to keep in mind that the BSM is a theoretical model when analysing the results.

6.1.1. Is the WOMBAT able to control the nitrogen levels effectively under stressed conditions?

Based on the BSM2 simulations, the WOMBAT® showed effective control under stressed weather conditions, where the effluent quality upper-limits were satisfied. Conversely, using the BSM1 gave nitrogen compound average values that violated the upper-limits. This could be due to the lower capacity of the aerobic and anoxic tanks in the biological reactor, where they were unable to cope with the large nitrogen compound load in the influent. We are inclined to prioritise the results from the BSM2 over the BSM1, since the BSM2 has a more complex set-up that resembles more closely an actual WWTP.

The Activated Sludge Model no. 1 (ASM1) describes the biological reactions, including the breakdown of nitrogen compounds in a reactor compartment of a WWTP. The ASM1 was linearised around the steady-state points provided by the BSM using the mean square method.

Stability of the linearised ASM1 was verified by observing the pole positions. This was to be expected, since the ASM1 is comprised of concentration equations. Concentrations in general are finite in real life, thus the aerobic and anoxic compartments always satisfy BIBO stability.

6.1.2. Is the WOMBAT in conjunction with the WWTP (robustly) stable?

Applying the BIBO stability theorem, it was deduced that the WWTP in conjunction with the WOMBAT® is stable. This was proved using the influent and effluent of the BSM simulations, where both were bounded (finite). Although this method of stability testing is not mathematically complex, it is considered sufficient and in fact more powerful than asymptotic stability. To test BIBO stability you can use non-zero influent values, whereas asymptotic stability uses zero influent values. Additionally, the simulations used a varied (non-zero) influent, containing rain, dry and storm weather condition data. Therefore, stability was verified through the simulation of multiple different real life influent scenarios.

We attempted to determine whether the system (with the WOMBAT® included) is robustly stable by applying the Additive Uncertainty model. Unfortunately, we were unable to derive the actual plant and consequently could not determine the robust stability. There may exist a simple way to find the actual plant of a WWTP, but we were unable to find any insightful research on this topic. Although, it could be argued that proof of robust stability is unnecessary, since the system acts stably (BIBO stable) for a wide range of weather conditions.

6.2. Recommendations

It is recommended when running the ASM, to update the linearisation during the simulation, taking live readings for linearisation points. The new linearised model is then able to adapt according to the concentrations in the actual compartment. This prevents the concentration values becoming negative and gives more simulation accuracy. Further, the simulations are not limited by high temperatures in the biological reactor. It is important that you update the linearised model enough during the simulation to anticipate sudden changes in concentrations.

It would be helpful to simulate the original non-linear ASM1 and compare the results against the results of the linearised ASM1. It is then possible to calculate the accuracy of the linearised ASM1 output.

For more insightful control simulations using the BSM2 set-up, it is advised for further analysis to reduce the size of the aerobic and anoxic compartments in the biological reactor. This should result generally in greater nitrogen compound levels during simulations, since the reduced capacity is less effective in dealing with break down of the nitrogen compound loads coming into the compartments. The WOMBAT® is then able to determine more frequently an oxygen set-point that is greater than 0.5 g (-COD)/m³ and thereby displaying how it copes with higher concentrations of nitrogen compounds.

Extremer conditions can be simulated using the BSM2 by modifying the temperature function, as seen in figure 6. For instance, increasing the amplitude of the sinusoidal temperature function gives a broader range of temperatures, leading to more challenging conditions for control. A lower temperature causes a decrease in the reaction rates in the aerobic compartment as seen in table 2. Therefore, the break down of nitrogen compounds is slower at lower temperatures. The extremer temperatures gives more insight into the control performance of the WOMBAT®, by revealing how the WOMBAT® copes when temperatures are exceptionally low or high in the aeration compartments.

In order to find robust stability of the WWTP in conjunction with the WOMBAT® controller, it may be possible to identify the *actual* plant by manually sweeping over a frequency range of interest in the WWTP using a signal generator. We were unable to find during our research a way to carry out this technique in an actual WWTP.

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Appendix A: WOMBAT[®]

This appendix contains confidential information about the WOMBAT[®] controller and is property of W+B. Please get in touch with W+B if you wish to gain access.

Appendix B: The Activated Sludge Model (ASM)

There are several versions of the activated sludge model (ASM). The models are comprised of mass-balance equations. The first and simplest version is the ASM1; published by the IAWQ (International Association on Water Quality) in 1986. The ASM1 describes organic matter degradation, nitrification and denitrification reactions. In 1995, the ASM2 was published; building on the ASM1 model by taking into account the biological phosphorus removal. The ASM2d was published in 1999 and includes denitrifying phosphorus-accumulation organisms, thereby giving a more accurate description of the dynamics of phosphate and nitrate. The ASM2d was closely followed by the ASM3. This model built on ASM1; incorporating additional sludge concepts. Including namely, detailed kinetic expressions of nitrogen and the dynamics of *storage polymers*. We have chosen to study the ASM1 in further depth, since ASM1 is the fundamental model and exhibits enough complexity for our analysis.

The 13 ASM1 states are displayed in table 5. A large portion of the states are measured in chemical oxygen demand (COD) units. This measures the amount of oxygen that can be consumed by reactions in a given solution. X denotes a particulate (biomass) component and S a soluble component. Observe that the units for S_O is minus COD, since it is the oxygen component and thus supplies oxygen rather than demanding it.

State	Description	Unit
S_I	Soluble inert organic matter	$M(COD)L^{-3}$
S_S	Readily biodegradable substrate	$M(COD)L^{-3}$
X_I	Particulate inert organic matter	$M(COD)L^{-3}$
X_S	Slowly biodegradable substrate	$M(COD)L^{-3}$
X_{BH}	Active heterotrophic biomass	$M(COD)L^{-3}$
X_{BA}	Active autotrophic biomass	$M(COD)L^{-3}$
X_P	Particulate products arising from biomass decay	$M(COD)L^{-3}$
S_O	Oxygen	$M(-COD)L^{-3}$
S_{NO}	Nitrate and nitrite	$M(N)L^{-3}$
S_{NH}	Ammonia and ammonium	$M(N)L^{-3}$
S_{ND}	Soluble biodegradable organic nitrogen	$M(N)L^{-3}$
X_{ND}	Particulate biodegradable organic nitrogen	$M(N)L^{-3}$
S_{ALK}	Alkalinity	Molar

Table 5: Overview of the states (components) in the ASM1. M stands for mass, COD for chemical oxygen demand, N for nitrogen and L for length. Taken from [9].

There are 8 different reactions in the ASM1 including: growth and decay of biomass (both heterotrophic and autotrophic), *ammonification* and *hydrolysis* [2]. The interactions are portrayed in figure 13. Note that the inert organic matter are not connected with the rest of the states, since they don't interact with other states. For simplicity, S_{ALK} and S_O are also not attached to the network, because they play a role in most of the reactions present [9].

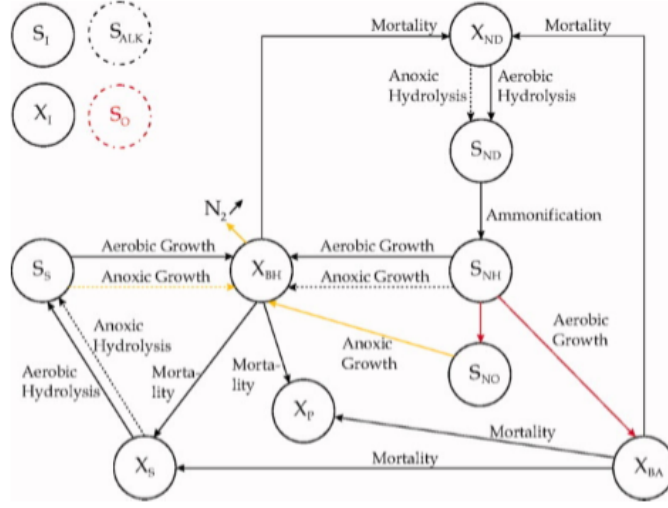


Figure 13: Interaction between the components in the ASM1. This image is taken from [6].

The ASM1 is comprised of the *kinetics* (rate-concentration dependence) and the *stoichiometry* (relationship that one component has on another in a reaction) of each wastewater process [2]. The ASM1 balance equations use the following standard structure:

$$\text{Input} - \text{Output} + \text{Reaction} = \text{Accumulation}$$

The system reaction term, r_i , is derived by summing the products of the stoichiometric coefficients ν_{ij} and the process rate expression ρ_j for the component i being considered in the mass balance:

$$r_i = \sum_j \nu_{ij} \rho_j$$

Further detail about the derivation of the equations can be found in the source [2]. The reactions are derived using the rates shown in table 6 with the corresponding stoichiometric terms displayed in table 7. It can be observed that the ASM1 consists of 13 reaction terms (balance equations). A table describing the stoichiometric parameters can be found in appendix A.

	Process	Process rate
ρ_1	Aerobic growth of heterotrophs	$\hat{\mu}_H \cdot \frac{S_S}{K_S + S_S} \cdot \frac{S_O}{K_{O,H} + S_O} \cdot X_{B,H}$
ρ_2	Anoxic growth of heterotrophs	$\hat{\mu}_H \cdot \frac{S_S}{K_S + S_S} \cdot \frac{K_{O,H}}{K_{O,H} + S_O} \cdot \frac{S_{NO}}{K_{NO} + S_{NO}} \cdot \eta_g \cdot X_{B,H}$
ρ_3	Aerobic growth of autotrophs	$\hat{\mu}_A \cdot \frac{S_{NH}}{K_{NH} + S_{NH}} \cdot \frac{S_O}{K_{O,A} + S_O} \cdot X_{B,A}$
ρ_4	Decay of heterotrophs	$b_H \cdot X_{B,H}$
ρ_5	Decay of autotrophs	$b_A \cdot X_{B,A}$
ρ_6	Ammonification of soluble organic nitrogen	$k_a \cdot S_{ND} \cdot X_{B,H}$
ρ_7	Hydrolysis of entrapped organics	$k_h \cdot \frac{X_S/X_{B,H}}{K_X + X_S/X_{B,H}} \cdot \left(\frac{S_O}{K_{O,H} + S_O} + \eta_h \cdot \frac{K_{O,H}}{K_{O,H} + S_O} \cdot \frac{S_{NO}}{K_{NO} + S_{NO}} \right) \cdot X_{B,H}$
ρ_8	Hydrolysis of entrapped organic nitrogen	$\rho_7 \cdot \frac{X_{ND}}{X_S}$

Table 6: Process rates of the ASM1. Taken from [9]. A description of the parameters can be found in table 8.

S_I	S_S	X_I	X_S	$X_{B,H}$	$X_{B,A}$	X_P	S_O	S_{NO}	S_{NH}	S_{ND}	X_{ND}	S_{ALK}	Process Rate, $\rho_j [ML^{-3}T^{-1}]$
	$\frac{-1}{Y_H}$			1			$\frac{-1+Y_H}{Y_H}$		$-i_{XB}$			$\frac{-i_{XB}}{14}$	ρ_1
	$\frac{-1}{Y_H}$			1			$\frac{-1+Y_H}{2.86Y_H}$		$-i_{XB}$			$\frac{1-Y_H}{14 \cdot 2.86Y_H} - \frac{i_{XB}}{14}$	ρ_2
					1		$\frac{-4.57+Y_A}{Y_A}$	$\frac{1}{Y_A}$	$-i_{XB} - \frac{1}{Y_A}$			$-\frac{i_{XB}}{14} - \frac{1}{7Y_A}$	ρ_3
			$1 - f_p$	-1		f_p					$i_{XB} - f_p i_{XP}$		ρ_4
			$1 - f_p$		-1	f_p					$i_{XB} - f_p i_{XP}$		ρ_5
									1	-1		$\frac{1}{14}$	ρ_6
	1		-1										ρ_7
										1	-1		ρ_8

Table 7: Stoichiometry matrix. Taken from [2].

Many of the rates in the ASM1 (shown in table 6) contain switch functions. These functions ensure that particular terms in the ASM equation appear or disappear when a concentration tends to zero.

An ASM1 balance equation can be derived by in table 7, looking along the column of one concentration, taking the derivative of the concentration (rate), setting it equal to the stoichiometry coefficient times the process rate (in the same row) and adding all the terms together. For example concentration S_O has the following balance equation:

$$\frac{dS_O}{dt} = \frac{-1 + Y_H}{Y_H} \rho_1 + \frac{-4.57 + Y_A}{Y_A} \rho_3$$

Parameter	Description	Type
Y_H	Heterotrophic yield	stoich.
Y_A	Autotrophic yield	stoich.
f_p	Fraction of biomass yielding particulate products	stoich.
i_{XB}	Mass of nitrogen per mass COD in biomass	stoich.
i_{XP}	Mass of nitrogen per mass COD in products of biomass	stoich.
μ_H	Heterotrophic maximum specic growth rate	kin.
b_H	Heterotrophic decay rate	kin.
K_S	Half-saturation coecient for heterotrophs	kin.
K_{OH}	Oxygen half-saturation coecient for heterotrophs	kin.
K_{NO}	Nitrate half-saturation coecient for denitrifying heterotrophs	kin.
μ_A	Autotrophic maximum specic growth rate	kin.
b_A	Autotrophic decay rat	kin.
K_{OA}	Oxygen half-saturation coecient for autotrophs	kin.
K_{NH}	Ammonia half-saturation coecient for autotrophs	kin.
η_g	Correction factor for anoxic growth of heterotroph	kin.
k_a	Ammonication rate	kin.
K_h	Maximum specic hydrolysis rate	kin.
K_X	Half-saturation coecient for hydrolysis of slowly biodegradable substrate	kin.
η_h	Correction factor for anoxic hydrolysis	kin.

Table 8: Description of the parameters in ASM1. Stoich. stands for stoichiometric and kin. for kinetic. Taken from [14].

Appendix C: State-space derivation and aeration compartment simulation (MATLAB®)

Linearised ASM1 reaction rates

The linear ASM1 reaction rates ρ_i are

$$\begin{aligned}\rho_1 &= a_{1,2}S_S + a_{1,5}X_{BH} + a_{1,8}S_O \\ \rho_2 &= a_{2,2}S_S + a_{2,5}X_{BH} + a_{2,8}S_O + a_{2,9}S_{NO} \\ \rho_3 &= a_{3,6}X_{BA} + a_{3,8}S_O + a_{3,10}S_{NH} \\ \rho_4 &= a_{4,5}X_{BH} \\ \rho_5 &= a_{5,6}X_{BA} \\ \rho_6 &= a_{6,5}X_{BH} + a_{6,11}S_{ND} \\ \rho_7 &= a_{7,4}X_S + a_{7,5}X_{BH} + a_{7,8}S_O + a_{7,9}S_{NO} \\ \rho_8 &= a_{8,5}X_{BH} + a_{8,8}S_O + a_{8,9}S_{NO} + a_{8,12}S_{ND}\end{aligned}$$

where $a_{i,j}$ is the parameter to be estimated. The index i stands for the reaction number and j for the rank of the variable in the state space vector \mathbf{z} .

Pole stability analysis

Verification that the poles lie in the left hand side plane of the complex plot can be seen in figure 14.

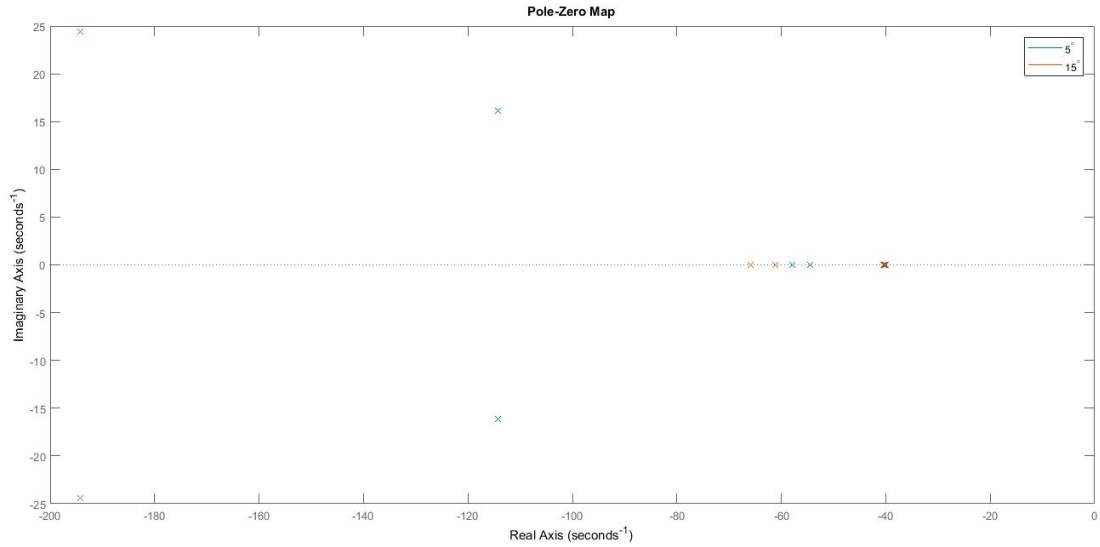


Figure 14: Aeration compartment state-space model pole plot at temperatures 15° and 5°. The plotted crosses represent the poles of the system.

Main linearisation script

```
1 %% Prep
2 close all; clc; clear all;
3
4 %% Data processing
```

```

5
6 % Fields of dataset: C1:t [6 hrs] C2:Si [g COD m-3] C3:Ss [g COD m-3] C4:Xi [g COD m-3]
7 % C5:Xs [g COD m-3] C6:Xbh [g COD m-3] C7:Xba [g COD m-3] C8:Xp [g COD
8 % m-3] C9:So [g -COD m-3]
9 % C10:Sno [g N m-3] C11:Snh [g N m-3] C12:Snd [g N m-3] C13:Xnd [g N
10 % m-3] C14:Salk [mole m-3] C15:Q [m3 d-1]
11 % Notes: S_O units -COD is equivalent to DO consumption
12 % Benchmark WWTP data extraction- Inf_rain_2006.txt
13 content = fileread('Inf_rain_2006.txt');
14 data_inf = textscan(content, '%f %f %f %f %f %f %f %f %f %f %f %f');
15
16 data_inf = [data_inf{2} data_inf{3} data_inf{4} data_inf{5} data_inf{6} data_inf{7}, ...
17 data_inf{8} data_inf{9} data_inf{10} data_inf{11} data_inf{12} data_inf{13} data_inf{14}
18 data_inf{15}];
19 % extend data for more detailed steps
20 data_inf_ext = zeros(6*length(data_inf)-5,14);
21 data_inf_ext(1,:) = data_inf(1,:);
22 up = 1;
23 data_pts = 6;
24 for j = 1:(length(data_inf)-1)
25     for i = 1:data_pts
26         data_inf_ext(i+up,:) = (i/data_pts).*(data_inf(j+1,:)-data_inf(j,:)) + data_inf(j,:);
27     end
28     up = up + 6;
29 end
30
31 %% Using BSM1 simulation set up
32 % Initial state space for aerobic tank
33 V = 1*1333; % [m3]
34 Q = 53377.6074; % Influent flow to AS %open-loop = 92230, closed-loop = 53377.6074
35 % Q/V = D (dilution rate)
36 T = 15; % [degrees] temperature of system
37 cut = 4000; % number of points to be erased
38
39 % Create time vector
40 content = fileread('Inf_rain_2006.txt');
41 data_inf1 = textscan(content, '%f %f %f %f %f %f %f %f %f %f %f %f');
42 data_inf1 = data_inf1{1};
43 t0 = zeros(6*length(data_inf1)-5,1);
44 t0(1) = data_inf1(1);
45 up = 1;
46 data_pts = 6;
47 for j = 1:(length(data_inf1)-1)
48     for i = 1:data_pts
49         t0(i+up,:) = (i/data_pts).*(data_inf1(j+1,1)-data_inf1(j,1)) + data_inf1(j,1);
50     end
51     up = up + data_pts;
52 end
53 t0 = t0(1:(end-cut));
54 label = ["S_I", "S_s", "X_I", "X_s", "X_{BH}", "X_{BA}", "X_p", "S_{NO}", "S_{NH}", "S_{ND}", "X_{ND}", "S_{ALK}"];
55 state_dim = length(label);
56
57 % Aerobic tank 5
58
59 % values inside reactor 5 from the BSM1 benchmark from WWTP simulation
60 % (steady state values)
61 SI_prox = 30; SS_prox = 0.80801; XI_prox = 1149.1683; % [mg COD/l]
62 XS_prox = 44.4828; XBH_prox = 2562.8514; XBA_prox = 154.163; % [mg COD/l]
63 XP_prox = 452.7367; % [mg COD/l]
64 SO_prox = 2; % [mg -COD/l]
65 SNO_prox = 13.5243; SNH_prox = 0.67193; SND_prox = 0.6645; XND_prox = 3.2605; % [mg N/l]
66 SALK_prox = 3.8277; % [mol HCO3/m3]
67
68 x0_aer5 = [SI_prox SS_prox XI_prox XS_prox XBH_prox XBA_prox XP_prox SO_prox SNO_prox SNH_prox
69 SND_prox XND_prox SALK_prox]; % tank initial condition (ensure no zero elements)
70 x0 = [30; 6.9; 46.95; 108.3; 133.2; 4.9; 0.036; 19.7; 11.5; 4; 4.8; 6.83];

```

```

70
71 [A1,B1,C1,D1,rho_aer5] = mean_squares_aer(x0_aer5,Q,V,T); % mean squares linearisation method
72 aer_tank5 = ss(A1,B1,C1,D1);
73
74 isstable(aer_tank5) % quick stability check [1=stable,0=not stable]
75
76 figure(180); clf;
77 pzmap(aer_tank5) % pole-zero map
78
79 set_pt = 2; % [mg/l] O2 set-point
80 data_len = length(data_inf_ext); % data length
81
82 inp = [data_inf_ext(:,1:7) data_inf_ext(:,9:13) set_pt*ones(data_len,1)];
83
84 adj = length(inp) - cut+1; % cut off excess data
85 inp(adj:end,:) = [];
86 y5 = lsim(aer_tank5,inp,t0',x0);
87
88 figure(85); %clf;
89 for i = 1:state_dim
90     subplot(4,3,i)
91     plot(t0,y5(:,i))
92     title(label(i))
93     hold on
94 end
95 hold on

```

Mean squares linearisation function

```

1 function [A1,B1,C1,D1,rho] = mean_squares_aer(x0,Q,V,T)
2 % Generates the state-space linearized model for given state x0
3
4 [Y_A,Y_H,f_p,i_XB,i_XE,i_XP,mu_H,K_s,K_OH,K_NO,b_A,b_H,eta_g,eta_h,k_h,K_x,mu_A,K_NH,K_OA,k_a] =
   ASM_param(T);
5
6 % define switch functions
7 Sub_switch1 = x0(2)/(K_s+x0(2));
8 NO_switch1 = x0(9)/(K_NO+x0(9));
9 O2_switch1 = x0(8)/(K_OH+x0(8));
10 O2_switch2 = K_OH/(K_OH+x0(8));
11 NH4_switch1 = x0(10)/(K_NH+x0(10));
12
13 % Process rates
14 rho1 = mu_H*Sub_switch1*O2_switch1*x0(5); % aerobic growth of heterotrophs rate
15 rho2 = mu_H*Sub_switch1*O2_switch2*NO_switch1*eta_g*x0(5); % anoxic growth of heterotrophs rate
16 rho3 = mu_A*NH4_switch1*O2_switch1*x0(6); % aerobic growth of autotrophs rate
17 rho4 = b_H*x0(5); % decay of heterotrophs rate
18 rho5 = b_A*x0(6); % decay of autotrophs rate
19 rho6 = k_a*x0(11)*x0(5); % ammonification of soluble organic nitrogen rate
20 rho7 = k_h*((x0(4)/x0(5))/(K_x+(x0(4)/x0(5))))*(O2_switch1+ eta_h*O2_switch2*NO_switch1)*x0(5); %
   hydrolysis of entrapped organics rate
21 rho8 = rho7*x0(12)/x0(4); % hydrolysis of entrapped organic nitrogen rate
22
23 rho = [rho1 rho2 rho3 rho4 rho5 rho6 rho7 rho8]';
24
25 M1 = [x0(2), x0(5), x0(8)];
26 M2 = [x0(2), x0(5), x0(8), x0(9)];
27 M3 = [x0(6), x0(8), x0(10)];
28 M6 = [x0(5), x0(11)];
29 M7 = [x0(4), x0(5), x0(8), x0(9)];
30 M8 = [x0(5), x0(8), x0(9), x0(12)];
31
32 theta1 = M1.\rho1; % finds coefficients [a12 a15 a18]
33 theta2 = M2.\rho2; % coefficients [a22 a25 a28 a29]
34 theta3 = M3.\rho3; % [a36 a38 a310]
35 theta4 = b_H; % a45
36 theta5 = b_A; % a56

```

```

37 theta6 = M6.\rho6; % [a65 a611]
38 theta7 = M7.\rho7; % [a74 a75 a78 a79]
39 theta8 = M8.\rho8; % [a85 a88 a89 a812]
40
41 phi = [0 theta1(1) 0 0 theta1(2) 0 0 theta1(3) 0 0 0 0 0; ...
42        0 theta2(1) 0 0 theta2(2) 0 0 theta2(3) theta2(4) 0 0 0 0; ...
43        0 0 0 0 0 theta3(1) 0 theta3(2) 0 theta3(3) 0 0 0; ...
44        0 0 0 0 0 theta4 0 0 0 0 0 0 0 0; ...
45        0 0 0 0 0 theta5 0 0 0 0 0 0 0; ...
46        0 0 0 0 0 theta6(1) 0 0 0 0 0 theta6(2) 0 0; ...
47        0 0 0 0 theta7(1) theta7(2) 0 0 theta7(3) theta7(4) 0 0 0 0; ...
48        0 0 0 0 theta8(1) 0 0 theta8(2) theta8(3) 0 0 theta8(4) 0];
49
50 W = [zeros(1,8); ...
51      -1/Y_H -1/Y_H zeros(1,4) 1 0; ...
52      zeros(1,8); ...
53      zeros(1,3) 1-f_p 1-f_p 0 -1 0; ...
54      1 1 0 -1 zeros(1,4); ...
55      0 0 1 0 -1 zeros(1,3); ...
56      zeros(1,3) f_p f_p zeros(1,3); ...
57      -(1-Y_H)/Y_H 0 (1- (4.57/Y_A)) zeros(1,5); ...
58      0 -(1-Y_H)/2.86*Y_H 1/Y_A zeros(1,5); ...
59      -i_XB -i_XB -i_XB-(1/Y_A) 0 0 1 0 0; ...
60      zeros(1,5) -1 0 1; ...
61      zeros(1,3) -i_XB-f_p*i_XB -i_XB-f_p*i_XB 0 0 -1; ...
62      -i_XB/14 ((1-Y_H)/142.86*Y_H)-i_XB/14 -(i_XB/14)-1/7*Y_A 0 0 1/14 0 0];
63 W(8,:) = [];
64 dim = length(W(:,1));
65
66 [ A1,B1,C1,D1 ] = state_space_gen_aer(Q,V,W,phi,dim );
67
68 end

```

ASM1 parameter derivation

```

1 function [Y_A,Y_H,f_p,i_XB,i_XE,i_XP,mu_H,K_s,K_OH,K_NO,b_A,b_H,eta_g,eta_h,k_h,K_x,mu_A,K_NH,
2          K_OA,k_a] = ASM_param(T)
3 % parameters for AS system at 15 degC, based on BSM1
4 mu_H = 4.0; %6.0;
5 K_s = 10.0; %20;
6 K_OH = 0.2;
7 K_NO = 0.5;
8 b_H = 0.3; %0.62;
9 mu_A = 0.5; %0.8;
10 K_NH = 1.0;
11 K_OA = 0.4;
12 b_A = 0.05; %0.2;
13 eta_g = 0.8;
14 k_a = 0.05; %0.08;
15 k_h = 3.0;
16 K_x = 0.1; %0.03;
17 eta_h = 0.8; %0.4;
18 Y_H = 0.67;
19 Y_A = 0.24;
20 f_p = 0.08;
21 i_XB = 0.08; %0.086;
22 i_XP = 0.06;
23 i_XE = i_XP;
24
25 mu_H = mu_H*exp((log(mu_H/3.0)/5.0)*(T-15.0)); /* Compensation from the current temperature in
26 the reactor */
27 b_H = b_H*exp((log(b_H/0.2)/5.0)*(T-15.0));
28 mu_A = mu_A*exp((log(mu_A/0.3)/5.0)*(T-15.0));
29 b_A = b_A*exp((log(b_A/0.03)/5.0)*(T-15.0));
30 k_h = k_h*exp((log(k_h/2.5)/5.0)*(T-15.0));
31 k_a = k_a*exp((log(k_a/0.04)/5.0)*(T-15.0));

```

31 end

State-space generation function

```
1 function [ A1,B1,C1,D1 ] = state_space_gen_aer(Q,V,W,phi,dim )
2 %State space generation
3 % kL_a = 10.26; % [1/hr] 240 [1/d] Mass transfer coefficient of the aeration equipment under the
   operating conditions imposed. 10 degrees values
4 % J = [zeros(7,1)' kL_a zeros(5,1)']';
5 J = [W*phi(:,8)]; % oxygen is taken to be the final input
6 phi(:,8) = [];
7 A = W*phi - ((Q/V)*eye(dim)); B = [(Q/V)*eye(dim) J];
8 C = eye(dim); D = zeros(dim,dim+size(J,2));
9
10 tank_ss = ss(A,B,C,D);
11 A1 = tank_ss.A;
12 B1 = tank_ss.B;
13 C1 = tank_ss.C;
14 D1 = tank_ss.D;
15
16 end
```

