

Composition Matrix and Conservation Equation

1. Stoichiometric Matrix

Convert molH to molH⁺ for protons

j	Process	Materials i				
		NH_4^+	O_2	NO_3^-	H_2O	H^+
		$\left[\frac{gNH_4 - N}{m^3} \right]$	$\left[\frac{gO_2}{m^3} \right]$	$\left[\frac{gNO_3 - N}{m^3} \right]$	$\left[\frac{molH_2O}{m^3} \right]$	$\left[\frac{molH}{m^3} \right]$
1	Nitrification	-1	ν_{O_2}	ν_{NO}	ν_{H_2O}	ν_H
	Unit of coefficient	$\left[\frac{gNH_4 - N}{gNH_4 - N} \right]$	$\left[\frac{gO_2}{gNH_4 - N} \right]$	$\left[\frac{gNO_3 - N}{gNH_4 - N} \right]$	$\left[\frac{molH_2O}{gNH_4 - N} \right]$	$\left[\frac{molH}{gNH_4 - N} \right]$

2. Composition Matrix

j	Process	Materials i				
		NH_4^+	O_2	NO_3^-	H_2O	H^+
		$\left[\frac{gNH_4 - N}{m^3} \right]$	$\left[\frac{gO_2}{m^3} \right]$	$\left[\frac{gNO_3 - N}{m^3} \right]$	$\left[\frac{molH_2O}{m^3} \right]$	$\left[\frac{molH}{m^3} \right]$
1	Nitrification	-1	ν_{O_2}	ν_{NO}	ν_{H_2O}	ν_H
k	Conservatives	Composition				
1	Nitrogen $\left[\frac{gN}{m^3} \right]$	1	0	1	0	0
	Unit of factor	$\left[\frac{gN}{gNH_4 - N} \right]$		$\left[\frac{gN}{gNO_3 - N} \right]$		
2	Oxygen $\left[\frac{gO}{m^3} \right]$	0	1	3.43	16	0
	Unit of factor		$\left[\frac{gO}{gO_2} \right]$	$\left[\frac{gO}{gNO_3 - N} \right]$	$\left[\frac{gO}{molH_2O} \right]$	
3	Hydrogen $\left[\frac{gH}{m^3} \right]$	0.29	0	0	2	1

	Unit of factor	$\left[\frac{gH}{gNH_4 - N} \right]$		$\left[\frac{gH}{molH_2O} \right]$	$\left[\frac{gH}{molH} \right]$	
4	Charge $\left[\frac{mol +}{m^3} \right]$	0.07	0	-0.07	0	1
	Unit of factor	$\left[\frac{mol +}{gNH_4 - N} \right]$		$\left[\frac{mol +}{gNO_3 - N} \right]$		$\left[\frac{mol +}{molH} \right]$

The key question that has to be answered is: "How much of the conservative element is included in the state variable?" In case of $l_{2,3}$ we ask: "How many grams of oxygen are associated with one gram of nitrate-nitrogen?" The composition factor $l_{2,3}$ is then calculated by rearranging equation (5.9):

$$l_{2,3} = \frac{C_{2,3}}{C_3} = \frac{3 \cdot 16 \frac{gO}{molNO_3}}{14 \frac{gNO_3 - N}{molNO_3}} = 3.43 \frac{gO}{gNO_3 - N}$$

Another illustrative example is the composition factor $l_{4,3}$:

$$l_{4,3} = \frac{C_{4,3}}{C_3} = \frac{-1 \frac{mol +}{molNO_3}}{14 \frac{gNO_3 - N}{molNO_3}} = -0.07 \frac{mol +}{gNO_3 - N}$$

3. Conservation Equations

In the nitrification reaction we have four unknown stoichiometric coefficients. We therefore need four conservation equations. We can write down four equations, one for each conservative element being part of the nitrification reaction, using equation (5.10):

Nitrogen: $-1 \cdot 1 + v_{NO} \cdot 1 = 0$

Oxygen: $v_{O_2} \cdot 1 + v_{NO} \cdot 3.43 + v_{H_2O} \cdot 16 = 0$

Hydrogen: $-1 \cdot 0.29 + v_{H_2O} \cdot 2 + v_H \cdot 1 = 0$

Charge: $-1 \cdot 0.07 + v_{NO} \cdot (-0.07) + v_H \cdot 1 = 0$

Solving the equation system for the four unknowns we get:

$$v_{O_2} = -4.57 \qquad v_{NO} = 1$$

$$v_{H_2O} = 0.0714 \qquad v_H = 0.143$$

4. Suitable Solution for Activated Sludge Systems

If we only want to use the conservation laws for TOD and nitrogen we are not able to calculate all stoichiometric coefficients any more. By considering also the conservation law for positive charge we are able to calculate three stoichiometric coefficients. In activated sludge models H_2O is usually not an interesting state variable. Thus, we can neglect this variable and reduce our stoichiometric coefficients to three.

Additionally we need the composition of the state variables in terms of TOD:

j	Process	Materials i			
		NH_4^+	O_2	NO_3^-	H^+
		$\left[\frac{gNH_4 - N}{m^3} \right]$	$\left[\frac{gO_2}{m^3} \right]$	$\left[\frac{gNO_3 - N}{m^3} \right]$	$\left[\frac{molH}{m^3} \right]$
1	Nitrification	-1	ν_{O_2}	ν_{NO}	ν_H
k	Conservatives	Composition			
5	TOD $\left[\frac{gTOD}{m^3} \right]$	0	-1	-4.57	0
Unit of factor			$\left[\frac{gTOD}{gO_2} \right]$	$\left[\frac{gTOD}{gNO_3 - N} \right]$	

Here $l_{5,2}$ and $l_{5,3}$ are calculated with table 5.8 and again equation (5.9) as:

$$l_{5,2} = \frac{C_{5,2}}{C_2} = \frac{2 \cdot (-16) \frac{gTOD}{molO_2}}{2 \cdot 16 \frac{gO_2}{molO_2}} = -1 \frac{gTOD}{gO_2}$$

$$l_{5,3} = \frac{C_{5,3}}{C_3} = \frac{(-24 - 3 \cdot 16 + 8) \frac{gTOD}{molNO_3}}{14 \frac{gNO_3 - N}{molNO_3}} = -4.57 \frac{gTOD}{gNO_3 - N}$$

The conservation equation for TOD is then:

$$\text{TOD: } \nu_{O_2} \cdot (-1) + \nu_{NO} \cdot (-4.57) = 0$$

Together with the conservation laws for nitrogen and charge the above system can be solved for the three unknown stoichiometric coefficients:

$$\nu_{O_2} = -4.57 \qquad \nu_{NO} = 1 \qquad \nu_H = 0.143$$

Conservation of TOD

1. Denitrification

The loss of nitrogen due to denitrification can be estimated from the conservation law on nitrogen:

$$N_{in} = N_{eff} + N_{acc} + N_{den}$$

with $N_{in} = i_N \cdot S_{COD,in} + S_{NH_4,in} + S_{NO_3,in} = 94.8 \text{g}_N/\text{m}^3$

$$N_{Eff} = i_N \cdot S_{COD,Eff} + S_{NH_4,Eff} + S_{NO_3,Eff} = 58.3 \text{g}_N/\text{m}^3$$

$$N_{Acc} = 10\% \cdot i_N \cdot S_{COD,in} = 1.3 \text{g}_N/\text{m}^3$$

$$N_{Den} = 35.2 \text{g}_N/\text{m}^3$$

2. Oxygen Consumption

Conservation of TOD: $S_{TOD,in} - S_{TOD,Eff} - S_{TOD,Acc} - S_{TOD,N_2} = S_{O_2}$

with $TOD_{NH_4} = 0 \text{g}_{TOD}/\text{g}_N$

$$TOD_{NO_3} = -4.57 \text{g}_{TOD}/\text{g}_N$$

$$TOD_{N_2} = -1.71 \text{g}_{TOD}/\text{g}_N$$

hence $S_{TOD,in} = S_{COD,in} + 0 \text{g}_{TOD}/\text{g}_N \cdot S_{NH_4,in} - 4.57 \text{g}_{TOD}/\text{g}_N \cdot S_{NO_3,in} = 320 \text{g}_{TOD}/\text{m}^3$

$$S_{TOD,Eff} = S_{COD,Eff} + 0 \text{g}_{TOD}/\text{g}_N \cdot S_{NH_4,Eff} - 4.57 \text{g}_{TOD}/\text{g}_N \cdot S_{NO_3,Eff} = -201.1 \text{g}_{TOD}/\text{m}^3$$

$$S_{TOD,Acc} = 10\% \cdot S_{COD,in} = 32 \text{g}_{TOD}/\text{m}^3$$

$$S_{TOD,N_2} = -1.71 \text{g}_{TOD}/\text{g}_N \cdot DN_{Den} = -60.2 \text{g}_{TOD}/\text{m}^3$$

$$S_{TOD,O_2} = 549.3 \text{g}_{O_2}/\text{m}^3$$

→ At least 2 m³ of air per m³ of wastewater must be supplied into the sand filter.

Breakpoint Chlorination: Stoichiometry and Composition

1. Stoichiometric and Composition Matrix

j	Process	Materials i								
		NH_4^+	$HOCl$	NH_2Cl	H_2O	H^+	$NHCl_2$	NCl_3	N_2	HCl
		[mol _{NH4+}]	[mol _{HOCl}]	[mol _{NH2Cl}]	[mol _{H2O}]	[mol _{H+}]	[mol _{NHCl2}]	[mol _{NCl3}]	[mol _{N2}]	[mol _{HCl}]
1	$NH_4^+ + HOCl \rightarrow NH_2Cl + H_2O + H^+$	-1	-1	1	1	1				
2	$NH_2Cl + HOCl \rightarrow NHCl_2 + H_2O$		-1	-1	1		1			
3	$NHCl_2 + HOCl \rightarrow NCl_3 + H_2O$		-1		1		-1	1		
4	$2NH_2Cl + HOCl \rightarrow N_2 + H_2O + 3HCl$		-1	-2	1				1	3
5	$NH_2Cl + NHCl_2 \rightarrow N_2 + 3HCl$			-1			-1		1	3
6	$3NH_2Cl + NCl_3 \rightarrow 2N_2 + 6HCl$			-1.5				-0.5	1	3
k	Conservatives *)	Composition								
1	Nitrogen [gN]	14		14			14	14	28	
	Unit of factor	$\left[\frac{gN}{mol_{NH_4}} \right]$		$\left[\frac{gN}{mol_{NH_2Cl}} \right]$			$\left[\frac{gN}{mol_{NHCl_2}} \right]$	$\left[\frac{gN}{mol_{NCl_3}} \right]$	$\left[\frac{gN}{mol_{N_2}} \right]$	
2	TOD [gTOD]	-	-16	-16	-	-	-32	-48	-48	-
	Unit of factor									

*) only the the conservatives, that are needed in the following tasks, are shown here.

2. TOD of Cl:

HCl is chosen as the species of Cl (comparable to NH₄⁺ for nitrogen), that has a TOD equal to 0. Therefore for Cl a TOD of “-8 gTOD mol_{Cl}⁻¹” results.

3. Composition matrix

The result is already presented in the task 1.

4. Conservation equation

The general form of the conservation equation looks as follow:

$$\sum_{i=1}^n v_{j,i} \cdot t_{k,i} = 0$$

i: composition factor

v: stoichiometric coefficient

i: number of the material

j: number of the process

k: number of the conservative substance

Now, we set up the equation for the **reaction 1**:

$$\begin{aligned} \text{N: } & v_{1,1} \cdot t_{1,1} + v_{1,2} \cdot t_{1,2} + v_{1,3} \cdot t_{1,3} + v_{1,4} \cdot t_{1,4} + v_{1,5} \cdot t_{1,5} = 0 \\ & (-1) \cdot 14 + (-1) \cdot 0 + 1 \cdot 14 + 1 \cdot 0 + 1 \cdot 0 = 0 \quad \checkmark \end{aligned}$$

$$\begin{aligned} \text{TOD: } & v_{1,1} \cdot t_{2,1} + v_{1,2} \cdot t_{2,2} + v_{1,3} \cdot t_{2,3} + v_{1,4} \cdot t_{2,4} + v_{1,5} \cdot t_{2,5} = 0 \\ & (-1) \cdot 0 + (-1) \cdot (-16) + 1 \cdot (-16) + 1 \cdot 0 + 1 \cdot 0 = 0 \quad \checkmark \end{aligned}$$

Reaction 4:

$$\begin{aligned} \text{N: } & v_{4,2} \cdot t_{1,2} + v_{4,3} \cdot t_{1,3} + v_{4,4} \cdot t_{1,4} + v_{4,8} \cdot t_{1,8} + v_{4,9} \cdot t_{1,9} = 0 \\ & (-1) \cdot 0 + (-2) \cdot 14 + 1 \cdot 0 + 1 \cdot 28 + 3 \cdot 0 = 0 \quad \checkmark \end{aligned}$$

$$\text{TOD: } (-1) \cdot (-16) + (-2) \cdot (-16) + 1 \cdot 0 + 1 \cdot (-48) + 3 \cdot 0 = 0 \quad \checkmark$$

Reaction 6:

$$\text{N: } (-1.5) \cdot 14 + (-0.5) \cdot 14 + 1 \cdot 28 + 3 \cdot 0 = 0 \quad \checkmark$$

$$\text{TOD: } (-1.5) \cdot (-16) + (-0.5) \cdot (-48) + 1 \cdot (-48) + 3 \cdot 0 = 0 \quad \checkmark$$

Deriving a Stoichiometric Matrix

1. Stoichiometric Matrix

From the reaction scheme the matrix in table 1 can be derived. The stoichiometric coefficients are calculated by setting the amount of the species that is reduced to -1 and then calculating the fraction that is converted from the reduced species into a specific product. An example is given for reaction 2, the Acidogenesis:

$$fraction_{am.acids_to_acetate} = \frac{Acetate_{of_total_COD}}{Am.acids_{of_total_COD}} = \frac{35\%}{66\%} = 0.53$$

As all the species are measured in gCOD the units of the stoichiometric coefficients are all 1 or gCOD/gCOD. The column of Part. Org. Material and the row of process o (Hydrolysis) should be seen as a summary of the three species that undergo Hydrolysis.

Table 1: Stoichiometric Matrix derived from the reaction scheme

j	Process	Materials i									
		Proteins	Carbohydrates	Lipids	Part. Org. Material	Aminoacids, sugars	Fatty acids	Interm. Products	Acetate	Hydrogen	Methane
		$\left[\frac{gCOD}{m^3}\right]$	$\left[\frac{gCOD}{m^3}\right]$	$\left[\frac{gCOD}{m^3}\right]$	$\left[\frac{gCOD}{m^3}\right]$	$\left[\frac{gCOD}{m^3}\right]$	$\left[\frac{gCOD}{m^3}\right]$	$\left[\frac{gCOD}{m^3}\right]$	$\left[\frac{gCOD}{m^3}\right]$	$\left[\frac{gCOD}{m^3}\right]$	$\left[\frac{gCOD}{m^3}\right]$
o	Hydrolysis	- 0.21	- 0.40	- 0.39	- 1						
iA	Hydrolysis	- 1				1					
iB	Hydrolysis		- 1			1					
iC	Hydrolysis			- 1		0.13	0.87				
2	Fermentation/ Acidogenesis					- 1		0.30	0.53	0.17	
3	Anaerobic Oxidation						- 1		0.68	0.32	
4	Fermentation/ Acetogenesis							- 1	0.6	0.4	
5	Acetotrophic Methanogenesis								- 1		1
6	Hydrogenotrophic Methanogenesis									- 1	1

2. Reconstruction of Reaction Scheme

Apart from the reaction between Acetate and Hydrogen that is marked with a question mark, the reaction scheme could exactly be reconstructed from the stoichiometric matrix. Thus no information was lost. However it would be necessary to have some process understanding (especially about the initial hydrolysis process and the way the composition of the raw sludge is expressed).

One problem in the reconstruction might be that this matrix and the reaction scheme do not deal with biomass and inert, non biodegradable organics.

3. Composition Matrix

As only the COD is important for this reaction scheme, the composition matrix only contains TOD as a conservative.

Table 2: Composition Matrix for the reaction scheme

		Materials i									
k	Conservatives	Proteins	Carbohydrates	Lipids	Part. Org. Material	Aminoacids, sugars	Fatty acids	Interm. Products	Acetate	Hydrogen	Methane
1	TOD	1	1	1	1	1	1	1	1	1	1
		$\left[\frac{gTOD}{gCOD} \right]$	$\left[\frac{gTOD}{gCOD} \right]$	$\left[\frac{gTOD}{gCOD} \right]$	$\left[\frac{gTOD}{gCOD} \right]$	$\left[\frac{gTOD}{gCOD} \right]$	$\left[\frac{gTOD}{gCOD} \right]$	$\left[\frac{gTOD}{gCOD} \right]$	$\left[\frac{gTOD}{gCOD} \right]$	$\left[\frac{gTOD}{gCOD} \right]$	$\left[\frac{gTOD}{gCOD} \right]$

4. Conservation of TOD

The reaction scheme assumes that the COD of the species involved in the reactions equals the TOD. COD is not a real conservative but in the scheme no COD is lost. The amount of all the species that are converted by the reactions is always given as the percentage of the COD that was available in the beginning, as particulate organic material. As TOD is a conservative the reactions convert 100% COD as particulate organic material into 100% COD as Methane.

Mass Balance in the Steady State

1. Dinitrogen exchange with atmosphere

In order to calculate the amount of dinitrogen, which is exchanged with the atmosphere, the total nitrogen in the inlet and in the outlet must be determined. The difference is the exchange with the atmosphere. So far we formulated the solution in words, in mathematical expression we get the following equations:

Mass balance for total nitrogen:

$$V \frac{\partial N_{tot}}{\partial t} = Q_{in} \cdot (c_{NH_4-N,in} + c_{N_2-N,in}) - Q_{out} \cdot (c_{NH_4-N,out} + c_{NO_3-N,out} + c_{N_2-N,out}) - R_{exchange} = 0 \quad (St.State)$$

Because there is no information about the inflow Q , it is only possible to calculate the fraction ($x_{exchange}$) of the inflow nitrogen that is exchanged with the atmosphere:

$$Q_{in} \cdot (c_{NH_4-N,in} + c_{N_2-N,in}) = 100\%$$

$$x_{exchange} = \frac{R_{exchange}}{Q_{in} \cdot (c_{NH_4-N,in} + c_{N_2-N,in})}$$

To be able to calculate this fraction we need to determine the exchange amount $R_{exchange}$.

$$R_{exchange} = Q \cdot \left(35 \frac{gN}{m^3}\right) - Q \cdot \left(32 \frac{gN}{m^3}\right) = Q \cdot 3 \frac{gN}{m^3}$$

$$x_{exchange} = \frac{Q \cdot 3 \frac{gN}{m^3}}{Q_{in} \cdot (c_{NH_4-N,in} + c_{N_2-N,in})} = 8.6\% \text{ which equals to } 3 \text{ gN m}^{-3} \text{ of wastewater.}$$

2. Oxygen transfer

By setting up a mass balance for the TOD the amount of oxygen, that is transferred to the wastewater, can be calculated. The difference of the TOD in the inflow and the outflow must be added to the wastewater by exchange with the atmosphere.

In Table 1 the calculation is shown. The second column includes the conversion factors to determine the TOD of all the compounds.

Table 1: Calculation of the TOD in the inflow and the outflow of the trickling filter in steady state.

Material	TOD	Inflow [$\text{g}_{\text{TOD}} \text{m}^{-3}$]	Outflow [$\text{g}_{\text{TOD}} \text{m}^{-3}$]	Stripping
O_2 [$\text{g}_{\text{O}_2} \text{m}^{-3}$]	- 1 [$\text{g}_{\text{TOD}} \text{g}_{\text{O}_2}^{-1}$]	- 2	- 6	? (unknown)
NH_4^+ [$\text{g}_\text{N} \text{m}^{-3}$]	0	-	-	
NO_3^- [$\text{g}_\text{N} \text{m}^{-3}$]	-4.57 [$\text{g}_{\text{TOD}} \text{g}_{\text{NO}_3\text{-N}}^{-1}$]	-	- 68.6	
N_2 [$\text{g}_\text{N} \text{m}^{-3}$]	-1.71 [$\text{g}_{\text{TOD}} \text{g}_{\text{N}_2\text{-N}}^{-1}$]	- 25.7	- 25.7	-5.13 *)
COD [$\text{g}_{\text{COD}} \text{m}^{-3}$]	1 [$\text{g}_{\text{TOD}} \text{g}_{\text{COD}}^{-1}$]	200	80	
Total TOD:		172.3	- 20.3	

*) From task 1 you get 3 $\text{g}_{\text{N}_2\text{-N}}$ per m^3 of wastewater that is stripped.

The result is now the difference of the TOD in the inflow and outflow plus the stripping. Therefore the TOD is reduced in the trickling filter by 197.7 g_{TOD} per m^3 wastewater. In other words 197.7 $\text{g}_{\text{O}_2} \text{m}^{-3}$ is transferred into the wastewater.

Ideal Reactors, Chemostats

1. Mass balances

The chemostat is modelled as a CSTR in steady state.

Mass balance for the substrate S_S :

$$V * \frac{dS_S}{dt} = Q * (S_{S,in} - S_S) + \left(-\frac{1}{Y_A} * \mu_A * \frac{S_S}{K_A + S_S} * X_A - \frac{1}{Y_B} * \mu_B * \frac{S_S}{K_B + S_S} * X_B \right) * V$$

$$\text{Steady state: } 0 = \frac{Q}{V} * (S_{S,in} - S_S) - \frac{1}{Y_A} * \mu_A * \frac{S_S}{K_A + S_S} * X_A - \frac{1}{Y_B} * \mu_B * \frac{S_S}{K_B + S_S} * X_B$$

Mass balance for organism A (X_A):

$$V * \frac{dX_A}{dt} = Q * (X_{A,in} - X_A) + \left(\mu_A * \frac{S_S}{K_A + S_S} * X_A - b_A * X_A \right) * V$$

$$\text{With } X_{A,in} = 0 \text{ and steady state: } 0 = 0 - \frac{Q}{V} * X_A + \left(\mu_A * \frac{S_S}{K_A + S_S} - b_A \right) * X_A$$

Mass balance for organism B (X_B):

$$V * \frac{dX_B}{dt} = Q * (X_{B,in} - X_B) + \left(\mu_B * \frac{S_S}{K_B + S_S} * X_B - b_B * X_B \right) * V$$

$$\text{With } X_{B,in} = 0 \text{ and steady state: } 0 = 0 - \frac{Q}{V} * X_B + \left(\mu_B * \frac{S_S}{K_B + S_S} - b_B \right) * X_B$$

2. Steady state solution with $Q = 1 \text{ l/d}$ and $S_{in} = 1000 \text{ gCOD/m}^3$.

Steady state solution for X_A :

$$0 = 0 - \frac{Q}{V} * X_A + \left(\mu_A * \frac{S_S}{K_A + S_S} - b_A \right) * X_A \quad /: X_A$$

$$\frac{Q}{V} + b_A = \mu_A * \frac{S_S}{K_A + S_S} \quad /* (K_A + S_S)$$

$$S_S(X_A) = \frac{-K_A * \left(\frac{Q}{V} + b_A \right)}{\left(\frac{Q}{V} + b_A - \mu_A \right)} = \frac{-5 \frac{\text{gCOD}}{\text{m}^3} * (1 \text{ d}^{-1} + 0.2 \text{ d}^{-1})}{1 \text{ d}^{-1} + 0.2 \text{ d}^{-1} - 6 \text{ d}^{-1}} = 1.25 \frac{\text{gCOD}}{\text{m}^3}$$

Steady state solution for X_B :

$$S_S(X_B) = \frac{-K_B * \left(\frac{Q}{A} + b_B\right)}{\left(\frac{Q}{V} + b_B - \mu_B\right)} = \frac{-50 \frac{\text{gCOD}}{\text{m}^3} * (1 \text{ d}^{-1} + 0.6 \text{ d}^{-1})}{1 \text{ d}^{-1} + 0.6 \text{ d}^{-1} - 12 \text{ d}^{-1}} = 7.69 \frac{\text{gCOD}}{\text{m}^3}$$

As organism X_B needs a higher steady state substrate concentration compared to organism X_A , organism X_B will be washed out under the given circumstances. Only organism X_A will survive in the chemostat.

The steady state biomass concentration of organism X_A can now be calculated with the steady state substrate concentration $S_S = 1.25 \text{ gCOD/m}^3$, assuming $X_B = 0$:

$$0 = \frac{Q}{V} * (S_{S,in} - S_S) - \frac{1}{Y_A} * \mu_A * \frac{S_S}{K_A + S_S} * X_A$$

$$X_A = \frac{(S_{S,in} - S_S) * (K_A + S_S)}{\frac{Q}{V} * \frac{1}{Y_A} * \mu_A * S_S} = \frac{(1000 - 1.25) \frac{\text{gCOD}}{\text{m}^3} * (5 + 1.25) \frac{\text{gCOD}}{\text{m}^3}}{1 \text{ d}^{-1} * \frac{1}{0.67} * 6 \text{ d}^{-1} * 1.25 \frac{\text{gCOD}}{\text{m}^3}} = 557.635 \frac{\text{gCOD}}{\text{m}^3}$$

Steady state solution with BM:

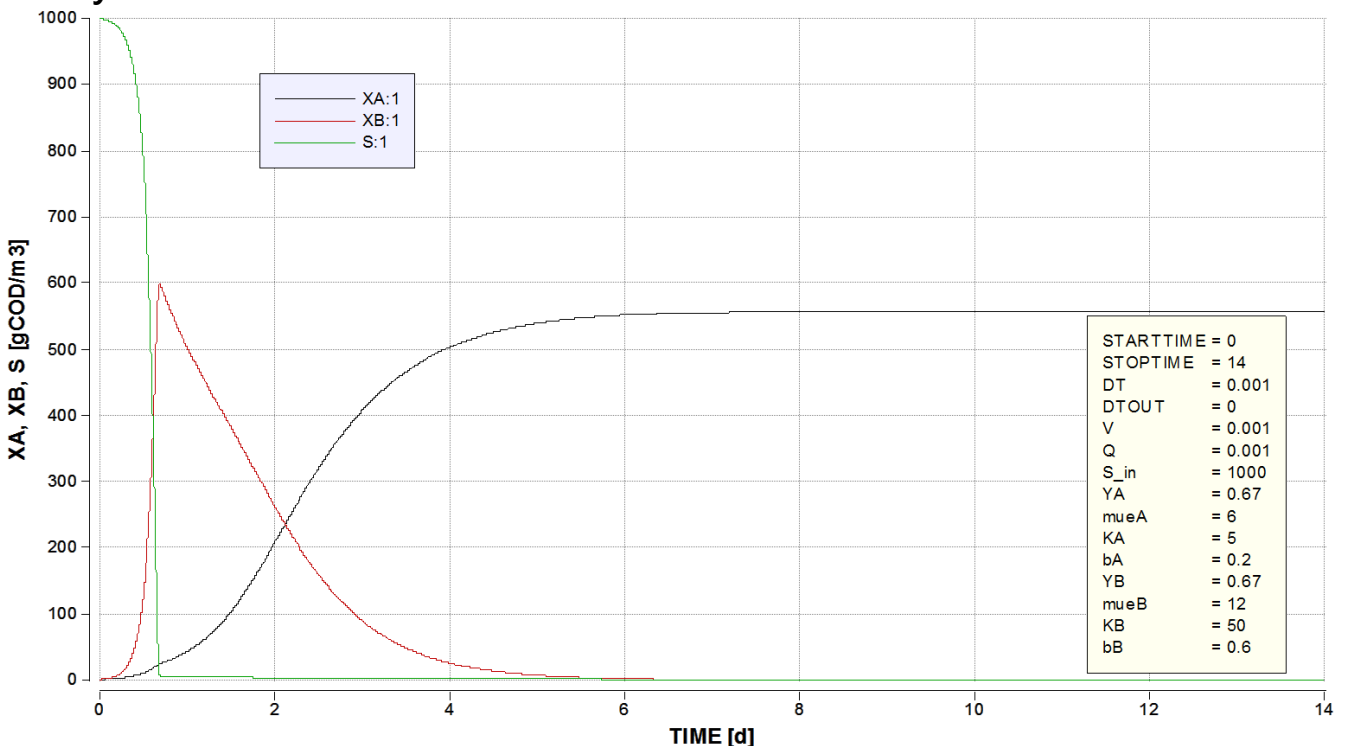


Figure 1: BM-solution for $Q = 0.001 \text{ m}^3/\text{d}$ and $S_{in} = 1000 \text{ gCOD/m}^3$.

After about 14 days, the steady state is reached: $X_A = 557.635 \text{ gCOD/m}^3$, $X_B = 4.103 \cdot 10^{-6} \text{ gCOD/m}^3$ and $S = 1.25 \text{ gCOD/m}^3$.

If we compare these results with the algebraic solution, we see in fact that the effluent substrate concentration corresponds to the steady state substrate concentration of X_A : $S_S(X_A) = 1.25 \text{ gCOD/m}^3$. Also, we can see that X_A dominates whereas X_B is washed out: The concentration of X_B is very small, whereas X_A reached steady state.

The reason for that lies in the K-value, which is the half-velocity constant. It indicates the substrate concentration at which a microorganism is at half the value of its maximum specific substrate utilization rate. Since microorganism A has a smaller K-value than B ($K_A = 5 \text{ gCOD/m}^3 < K_B = 50 \text{ gCOD/m}^3$), it follows that A dominates at lower substrate concentrations. Although X_B has a faster growth rate ($\mu_B = 12 \text{ d}^{-1} > \mu_A = 6 \text{ d}^{-1}$), which can be seen in the early peak of the X_B concentration (see Figure 1), it declines very rapidly as soon as the substrate concentration in the reactor diminishes. As soon as X_B declines, the concentration of X_A rises until it reaches its steady state value.

3. Changing the substrate concentration in the influent

The influence of a changing influent substrate concentration on the biomass composition can be seen in Figure 2, whereas the influence on the effluent substrate concentration is depicted in Figure 3.

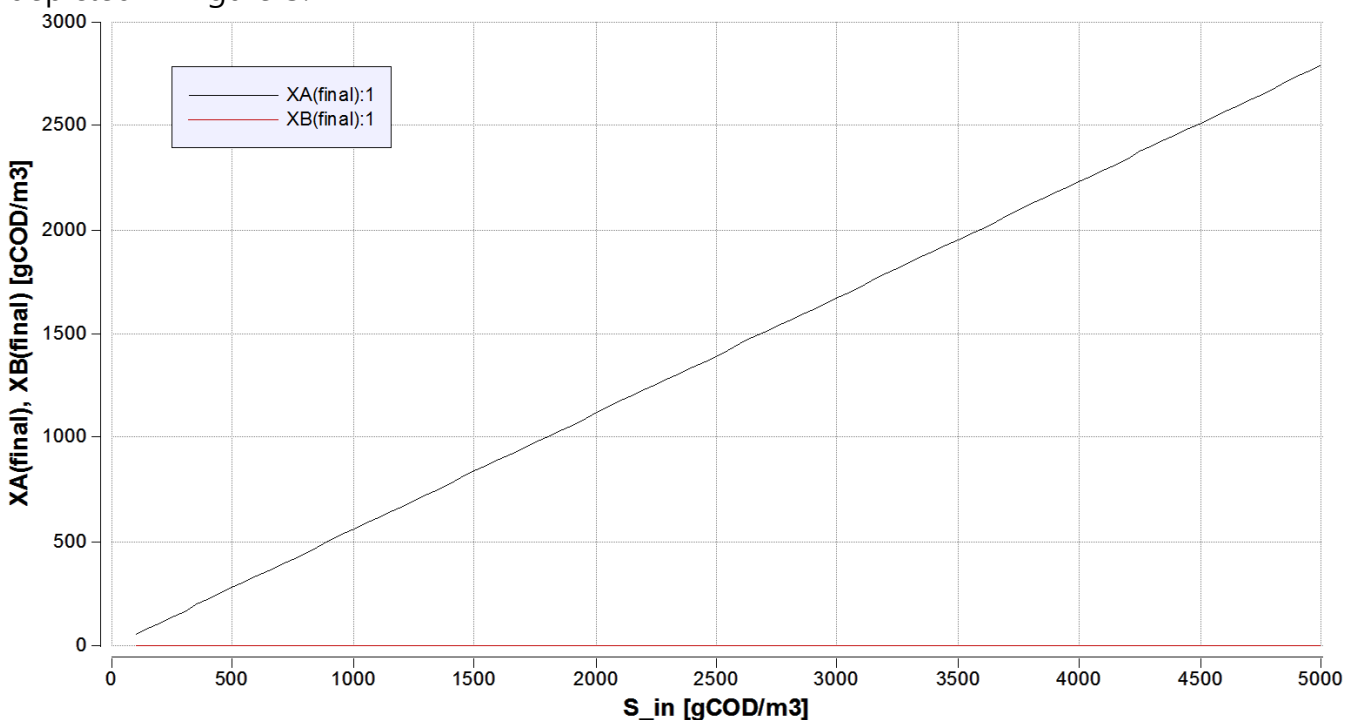


Figure 2: Parameter plot of the biomass composition for $S_{S,in} = 100\text{-}5000 \text{ gCOD/m}^3$ while keeping the flow rate Q constant at $0.001 \text{ m}^3/\text{d}$.

A variation of the influent substrate concentration does not change the situation fundamentally: over the whole indicated range, X_A still dominates compared to X_B . The same can be seen as well when the relative share of X_A and X_B in the total biomass are plotted.

The effluent substrate concentration stays at its steady state value of 1.25 gCOD/m^3 as it is independent of $S_{S,in}$ (see Figure 3).

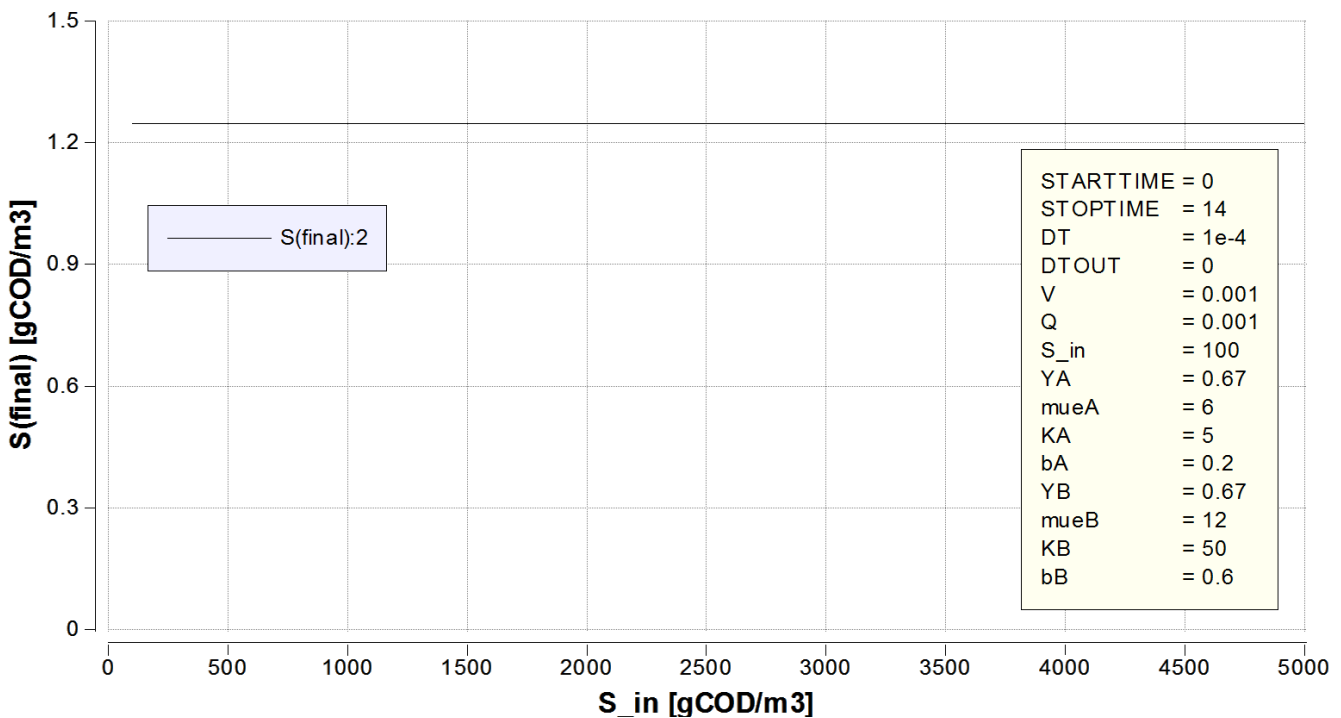


Figure 3: Parameter plot of the effluent substrate concentration for $S_{S,in} = 100\text{-}5000 \text{ gCOD/m}^3$ while keeping the flow rate Q constant at $0.001 \text{ m}^3/\text{d}$.

4. Changing the flow rate Q

If the influent Q is increased but $S_{S,in}$ is held constant, there is in total more substrate flowing into the reactor, as the load increases. Between influent values of 0.0046 and $0.0052 \text{ m}^3/\text{s}$, the concentration of X_A starts to decrease and microorganism B starts to dominate. Unlike the situation in subtask 3, the effluent substrate concentration in Figure 5 rises enormously because the substrate is being accumulated in the chemostat. The microorganisms are not able to cope with the high influent load anymore.

The increase in load can not be the explanation to these observations, as the load increases in subtask 3, too. The main difference between the situation in subtask 3 and the one in subtask 4 is the increased hydraulic disturbance. For $Q = 0.001 \text{ m}^3/\text{d}$ and $S_{S,in} = 5000 \text{ gCOD}/\text{d}$, the mean hydraulic residence time is 1 d ($\theta_h = V/Q$), whereas e.g. for $Q = 0.0046 \text{ m}^3/\text{d}$ and $S_{S,in} = 1000 \text{ gCOD}/\text{d}$, it is only 0.22 d. As the flow rate increases, the hydraulic residence time decreases (see Figure 6) and the microorganisms are washed out, first organism A and then also B (see Figure 4).

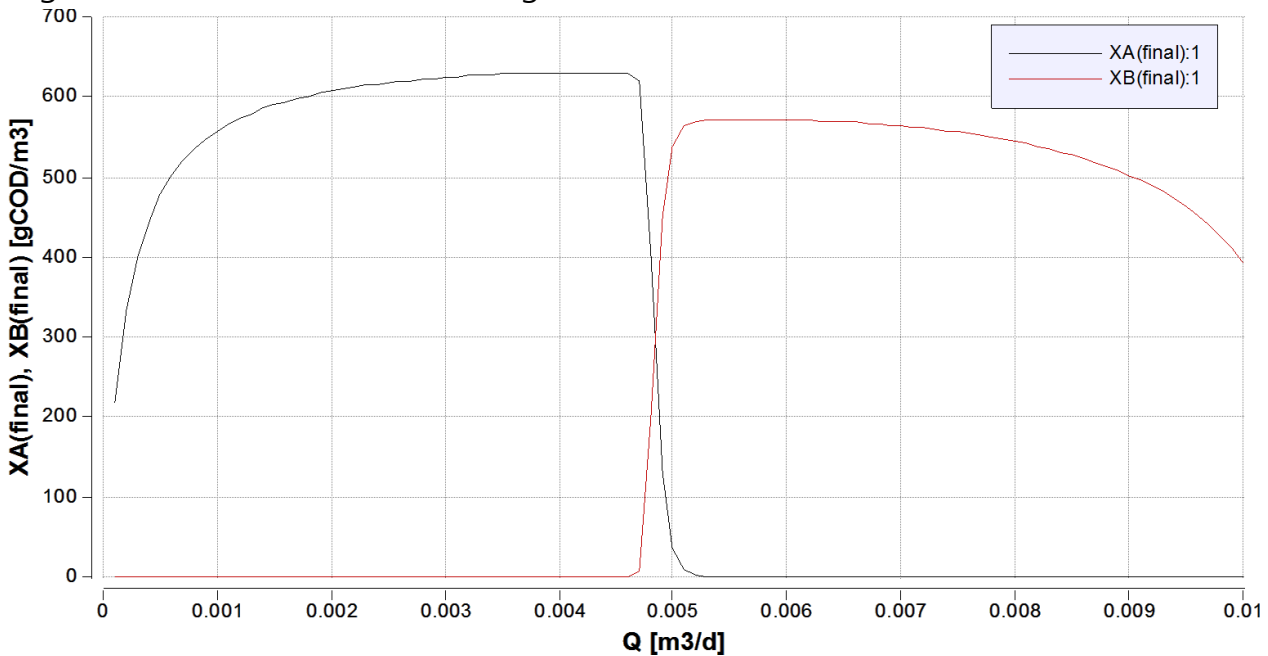


Figure 4: Parameter plot of the biomass composition for $Q = 0.0001-0.01 \text{ m}^3/\text{d}$ while keeping $S_{S,in}$ constant at $1000 \text{ gCOD}/\text{m}^3$.

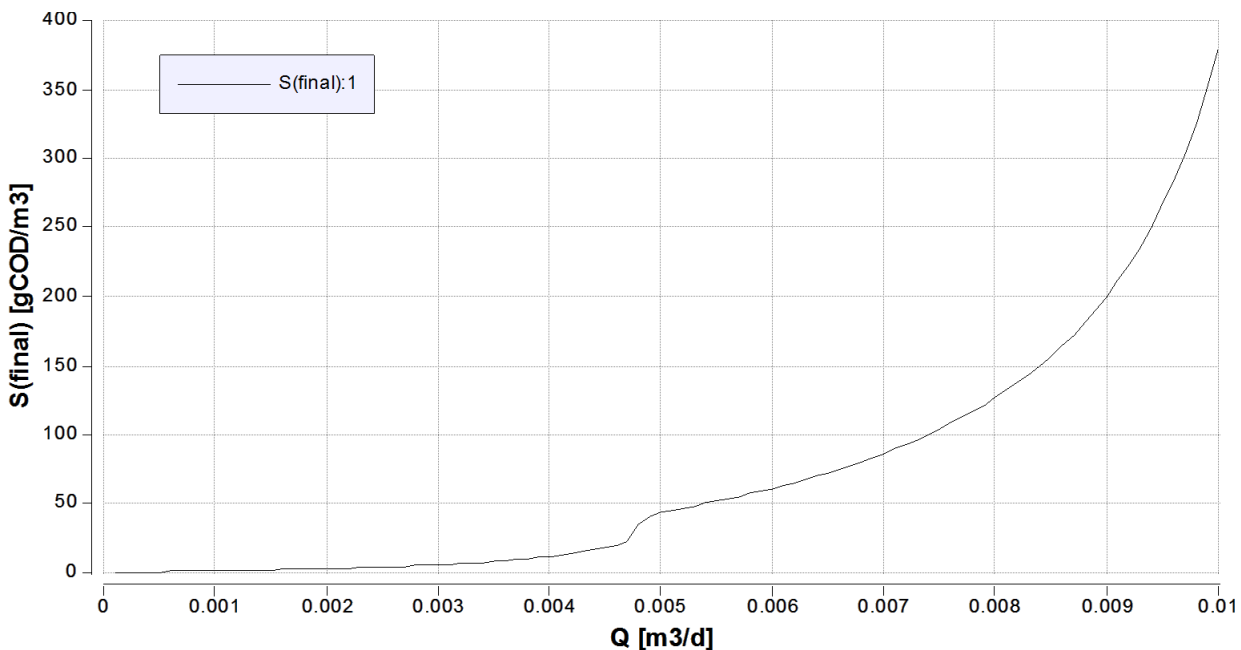


Figure 5: Parameter plot of the effluent substrate concentration for $Q = 0.0001-0.01 \text{ m}^3/\text{d}$ while keeping $S_{S,in}$ constant at $1000 \text{ gCOD}/\text{m}^3$.

The washout of microorganisms happens if the hydraulic residence time θ_h becomes smaller than the organism's minimal solids retention time $\theta_{x,min}$ (Note: for CSTR in steady state, without return sludge $\rightarrow \theta_h = \theta_x$):

$$\text{Washout for } \theta_h < \theta_{x,min} = \frac{K + S_{in}}{S_{in} * (\mu_m - b) - b * K}$$

For a given influent substrate concentration, microorganism A has a lower $\theta_{x,min}$ than B and is therefore washed out first (see Figure 6).

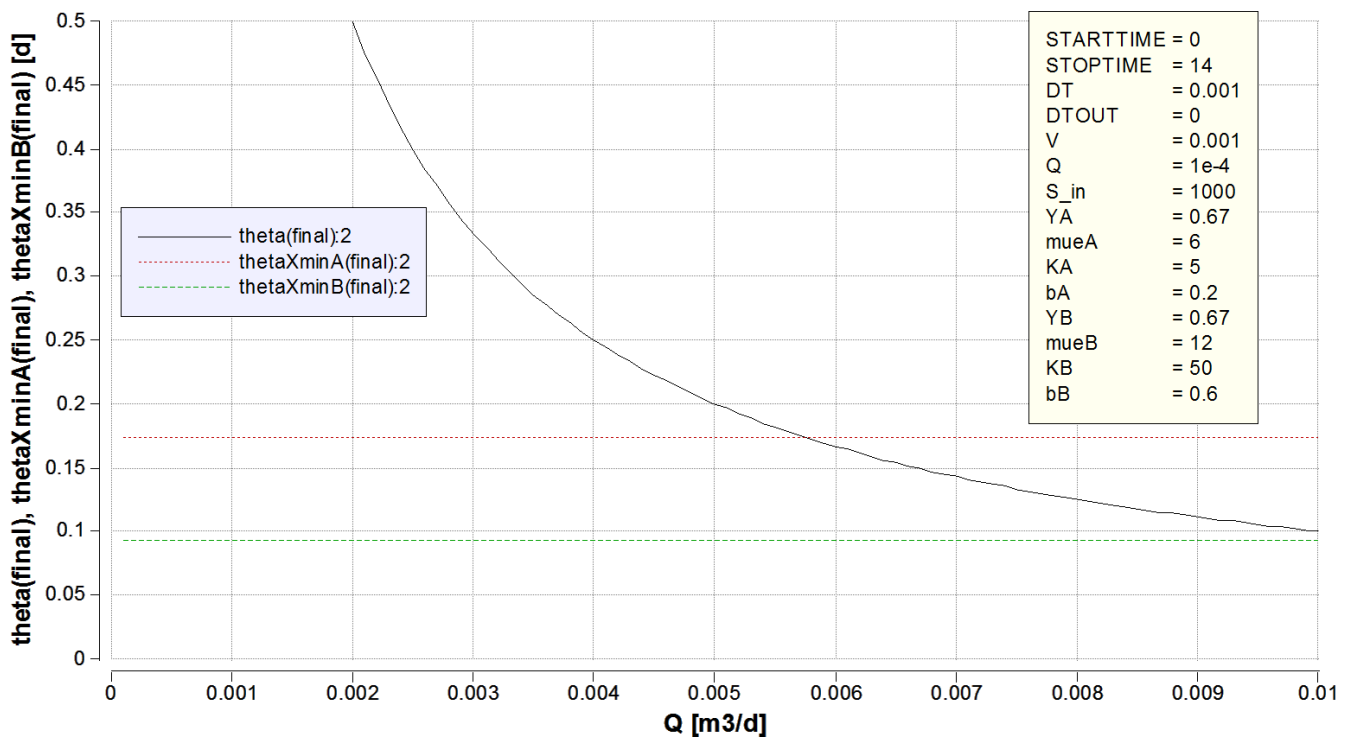


Figure 6: Parameter plot of the hydraulic residence time and the minimal solids retention times for A and B, respectively; for $Q = 0.0001-0.01 \text{ m}^3/\text{d}$ and $S_{S,in} = 1000 \text{ gCOD}/\text{m}^3 = \text{constant}$ (Y-axis cut for better visibility of the graphs, θ_h starts at 10 d).

The hydraulic residence time does obviously not change while changing $S_{S,in}$. With a constant θ_h of 1 d in subtask 3, neither $\theta_{x,min,A}$ (0.1733 to 0.1726 d) nor $\theta_{x,min,B}$ (0.0923 to 0.0886 d) is reached. Therefore microorganism A is more competitive over the whole range of $S_{S,in}$ because it requires a lower substrate concentration in the reactor.

It can be concluded that microorganism B is more competitive in terms of the solids retention time, whereas microorganism A is more competitive in terms of the minimal required substrate concentration in the reactor.

Ideal Reactors, Plug Flow

1. Mass balances

According to Streeter and Phelps (1925) it is assumed that very large rivers can be modelled with an ideal plug-flow in steady state.

The required mass balances for dissolved oxygen and the pollutant BOD are shown below.

Oxygen:

$$\frac{\partial S_O}{\partial t} = -\frac{\partial S_O}{\partial \tau} - K_1 * C_S + K_2 * (S_{O,sat} - S_O)$$

$$\text{with } d\tau = \frac{dx}{u} \text{ and } r_{SO} = -K_1 * C_S + K_2 * (S_{O,sat} - S_O)$$

$$\text{In steady state: } \frac{\partial S_O}{\partial t} = 0 \rightarrow \frac{\partial S_O}{\partial \tau} = r_{SO} \text{ or } \frac{\partial S_O}{\partial x} = \frac{1}{u} * r_{SO}$$

BOD:

$$\frac{\partial C_S}{\partial t} = -\frac{\partial C_S}{\partial \tau} - K_1 * C_S \text{ with } d\tau = \frac{dx}{u}$$

$$\text{In steady state: } \frac{\partial C_S}{\partial t} = 0 \rightarrow \frac{\partial C_S}{\partial \tau} = -K_1 * C_S \text{ or } \frac{\partial C_S}{\partial x} = \frac{1}{u} * (-K_1 * C_S)$$

2. Length profile of BOD and oxygen concentration along the river

In Figure 1, the total river length was assumed to be around 1000 km. The steady state concentrations are reached asymptotically.

S_O decreases to a minimal value until it rises again to the saturation value ($9 \text{ gO}_2/\text{m}^3$). The BOD concentration, C_S , decreases exponentially.

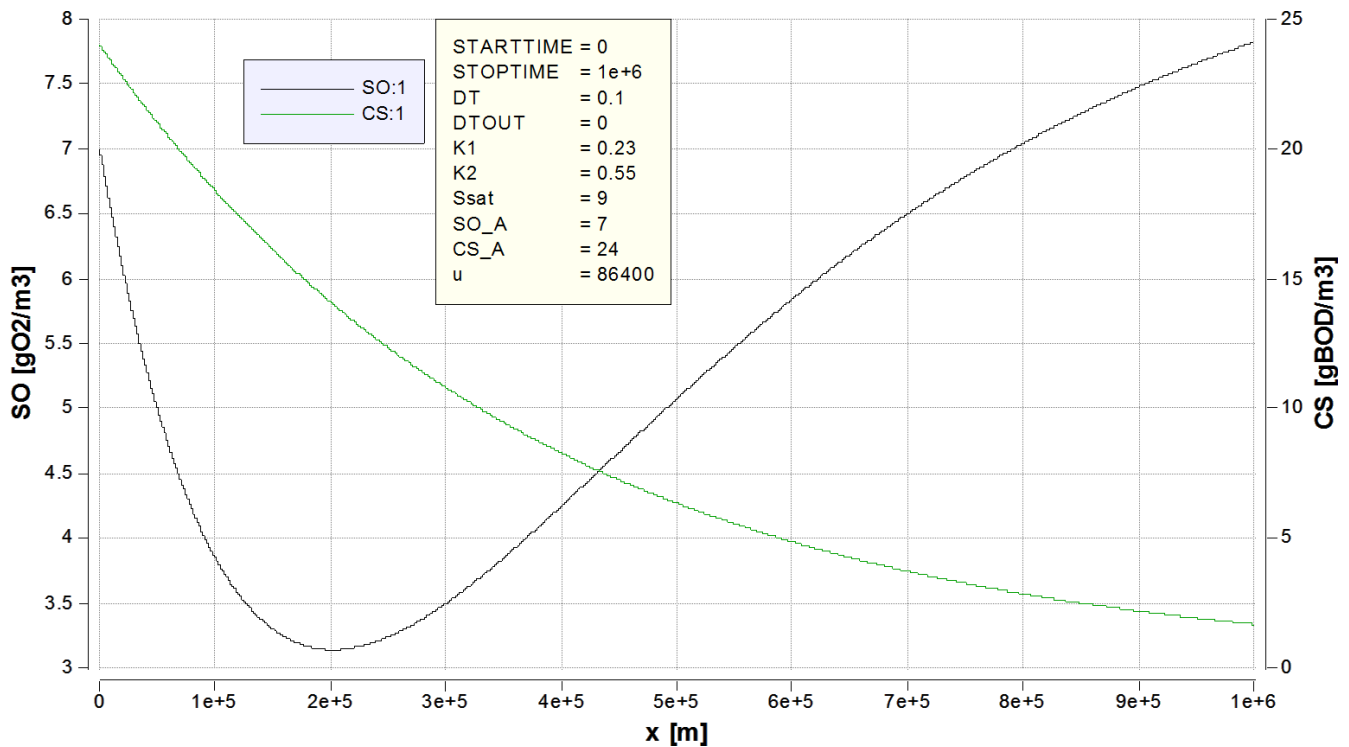


Figure 1: Length profile of the BOD concentration and the oxygen concentration along a river length of 1000 km, starting at location A (= x_0), with a mean flow velocity $u = 1$ m/s.

4. Minimal oxygen concentration

For the given parameter set, the location at which the dissolved oxygen reaches a minimum ($S_{O,min}$) is at a river length of about 200 km.

However, the location of $S_{O,min}$ depends on the expression for the rate in the mass balance, $r_{SO} = -K_1 \cdot C_S + K_2 \cdot (S_{sat} - S_O)$, where $-K_1 \cdot C_S$ describes degradation and $K_2 \cdot (S_{sat} - S_O)$ accounts for reaeration. The rate determines if S_O' ($= dS_O/dx$) is positive or negative. As long as degradation $>$ reaeration, S_O' is negative and S_O decreases; as soon as degradation $<$ reaeration, S_O' turns positive and S_O starts to increase.

The location of $S_{O,min}$ depends mainly on the kinetic parameters K_1 and K_2 , the oxygen saturation value S_{sat} and also on the initial conditions for S_O and C_S . The faster the kinetic processes, the sooner the minimal oxygen concentration is reached.

This can also be seen with the help of a simple sensitivity analysis. The following plots show the change of the location for $S_{O,min}$ if the value for one parameter is either halved or doubled while keeping the values for the other parameters (including the initial conditions) constant:

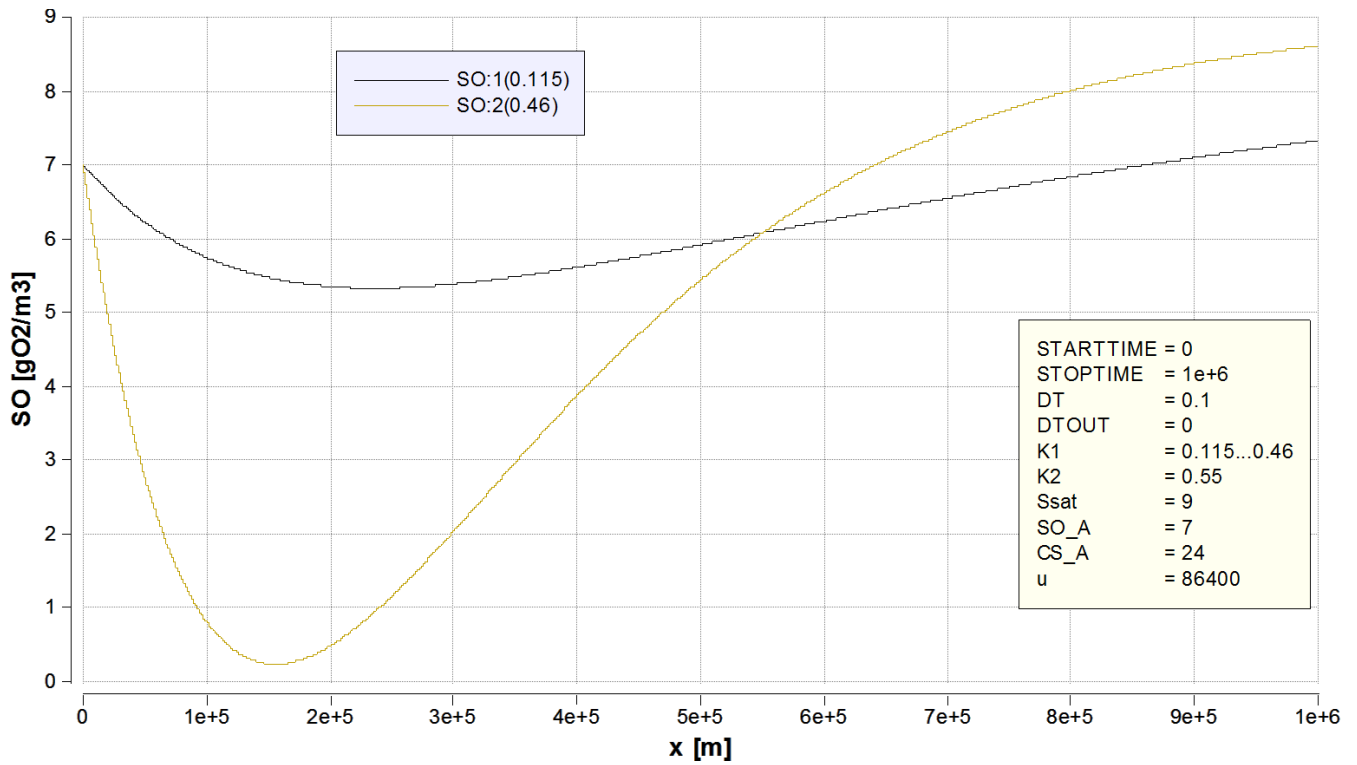


Figure 2: Sensitivity of the oxygen concentration to a variation of parameter K_1 (degradation).

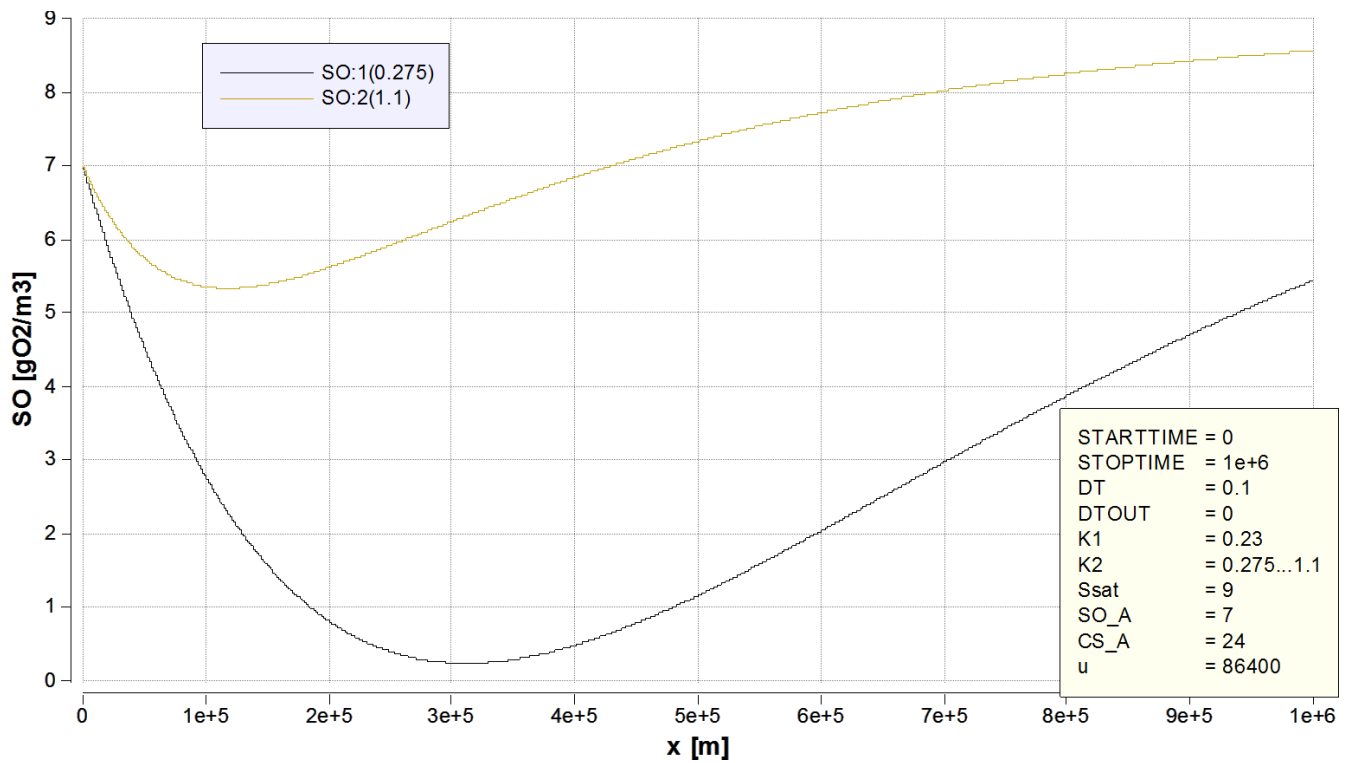


Figure 3: Sensitivity of the oxygen concentration to a variation of parameter K_2 (reaeration).

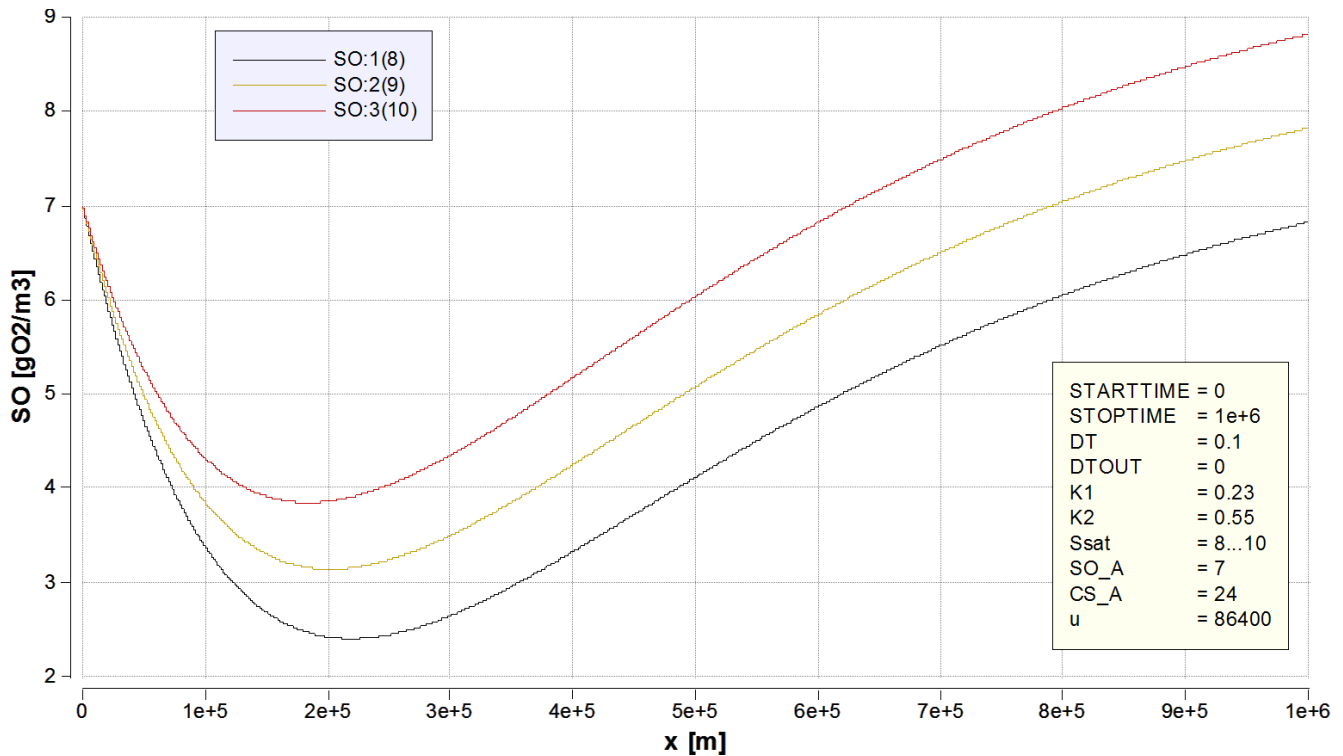


Figure 4: Sensitivity of the oxygen concentration to a variation of parameter S_{sat} .

5. Model: ideal plug-flow reactor

In order to judge if the model of an ideal plug-flow reactor is justified for the application for very large rivers, the extent of dispersion is a crucial property. The longitudinal dispersion coefficient of a river can be estimated with the help of Table 4.4:

Assumptions:

$$u^* \approx 0.075 \cdot v = 0.075 \text{ m/s}$$

$$b \approx 100 \text{ m}$$

$$h \approx 3 \text{ m}$$

$$\rightarrow D_{D,x} = 0.011 \cdot \frac{v^2 \cdot b^2}{h \cdot u^*} = 0.011 \cdot \frac{\left(1 \frac{\text{m}}{\text{s}}\right)^2 \cdot (100 \text{ m})^2}{3 \text{ m} \cdot 0.075 \frac{\text{m}}{\text{s}}} = 488.9 \frac{\text{m}^2}{\text{s}} = 42'240'000 \frac{\text{m}^2}{\text{d}}$$

The turbulence number for e.g. $L = 200 \text{ km}$ is therefore:

$$N_T = \frac{D_T}{u \cdot L} = \frac{489 \frac{\text{m}^2}{\text{s}}}{1 \frac{\text{m}}{\text{s}} \cdot 200'000 \text{ m}} = 0.0025$$

The turbulence number compares the relevance of turbulence and of advection in a given system and is defined as:

$$N_T = \frac{\text{relevance of turbulence}}{\text{relevance of advection}}$$

So if $N_T < 1$, advection outweighs dispersion. For the system under investigation, advection is about 400 times more important than dispersion, which justifies the assumption of an ideal plug-flow reactor without turbulence.

Ideal Reactors, Sampling in Turbulent Flow

1. Material balance equations for oxygen

The aeration tank can be modelled as a plug-flow reactor with turbulence. The stationary material balances for the three sections can be set up as follows:

Section x_1 (0 m) to x_2 (20 m):

$$0 = Q * (S_{O,in} - S_{O,20}) + D_T * A * \left. \frac{dS_O}{dx} \right|_{x_2} + (r_{O,Av,1-2} + k_l a * (S_{O,sat} - S_{O,Av,1-2})) * A * (x_2 - x_1)$$

Section x_2 (20 m) to x_3 (40 m):

$$0 = Q * (S_{O,20} - S_{O,40}) + D_T * A * \left(- \left. \frac{dS_O}{dx} \right|_{x_2} + \left. \frac{dS_O}{dx} \right|_{x_3} \right) + (r_{O,Av,2-3} + k_l a * (S_{O,sat} - S_{O,Av,2-3})) * A * (x_3 - x_2)$$

Section x_3 (40 m) to x_4 (60 m):

$$0 = Q * (S_{O,40} - S_{O,out}) - D_T * A * \left. \frac{dS_O}{dx} \right|_{x_3} + (r_{O,Av,3-4} + k_l a * (S_{O,sat} - S_{O,Av,3-4})) * A * (x_4 - x_3)$$

2. Estimation of the average oxygen consumption rate, $r_{O,Av}$

Per definition, the oxygen consumption rate is negative: $r_O < 0$.

The oxygen concentrations gradients $\frac{dS_O}{dx}$ can be determined from the length profile of the oxygen concentration:

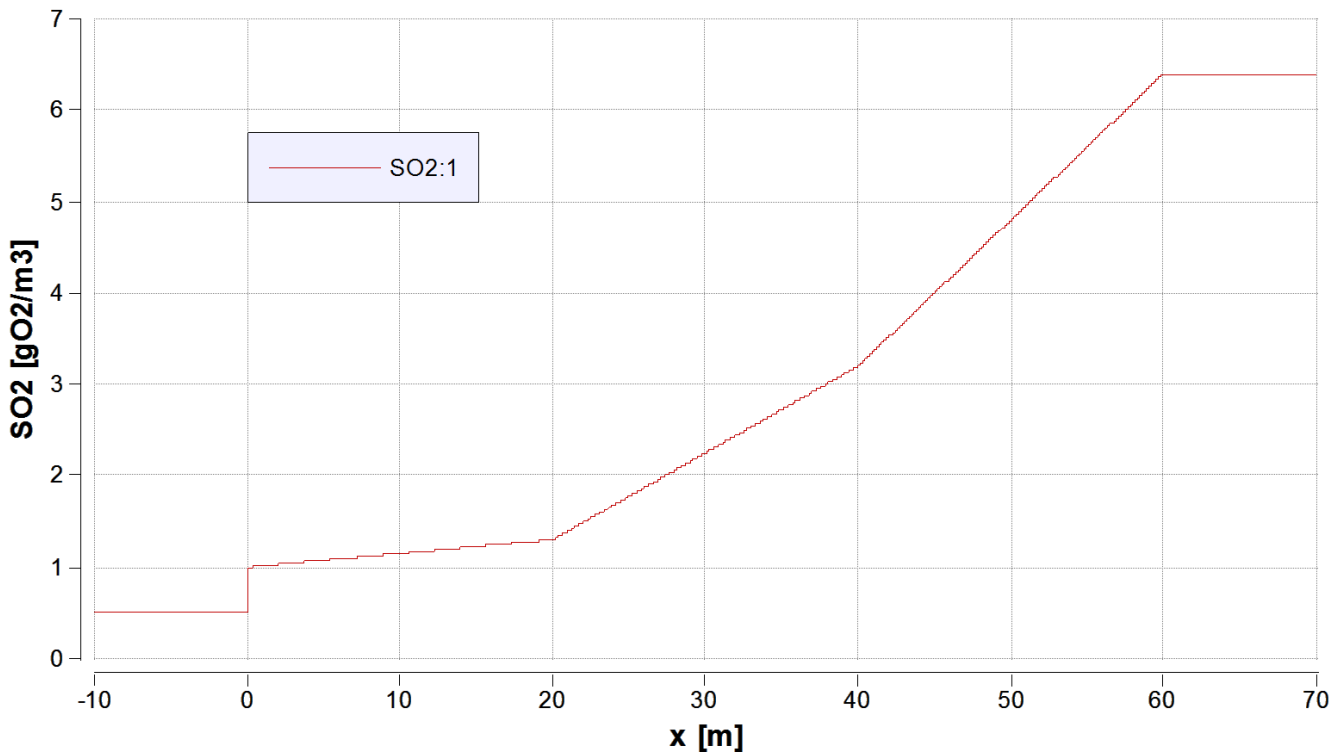


Figure 1: Length profile of the oxygen concentration (increasing because of reaeration).

Estimated concentration gradients with the help of Figure 1 (Note: values determined by linear interpolation):

$$\left. \frac{dS_O}{dx} \right|_{x_2} = 0.0625 \frac{gO_2}{m^4}$$

$$\left. \frac{dS_O}{dx} \right|_{x_3} = 0.125 \frac{gO_2}{m^4}$$

Calculation of oxygen consumption rates in the three compartments:

Section x_1 to x_2 :

$$r_{O,Av,1-2} = \left(-4800 \frac{m^3}{d} * (0.5 - 1.3) \frac{gO_2}{m^3} - 24'000 \frac{m^2}{d} * 24 m^2 * 0.0625 \frac{gO_2}{m^4} \right) * \frac{1}{24 m^2 * 20 m} - 50 d^{-1} * \left(10 - \left(\frac{1.3 + 0.5}{2} \right) \right) \frac{gO_2}{m^3} = -522.0 \frac{gO_2}{m^3 * d}$$

Section x_2 to x_3 :

$$r_{O,Av,2-3} = \left(-4800 \frac{m^3}{d} * (1.3 - 3.2) \frac{gO_2}{m^3} - 24'000 \frac{m^2}{d} * 24 m^2 * \left(-0.0625 \frac{gO_2}{m^4} + 0.125 \frac{gO_2}{m^4} \right) \right) * \frac{1}{24 m^2 * 20 m} - 50 d^{-1} * \left(10 - \left(\frac{3.2 + 1.3}{2} \right) \right) \frac{gO_2}{m^3} = -443.5 \frac{gO_2}{m^3 * d}$$

Section x₃ to x₄:

$$r_{O,Av,3-4} = \left(-4800 \frac{m^3}{d} * (3.2 - 6.4) \frac{gO_2}{m^3} + 24'000 \frac{m^2}{d} * 24 m^2 * 0.125 \frac{gO_2}{m^4} \right) * \frac{1}{24 m^2 * 20 m} \\ - 50 d^{-1} * \left(10 - \left(\frac{6.4 + 3.2}{2} \right) \right) \frac{gO_2}{m^3} = -78.0 \frac{gO_2}{m^3 * d}$$

3. Improvement of this experiment

- Determine the exact concentration gradients $\frac{dS_O}{dx}$ at the sampling points.
- For subtask 2, a linear curve for the oxygen consumption between the sampling points was assumed, since $\frac{dS_O}{dx}$ was not available. But in a PFR, the length profile of the degradation / consumption curve of a material is rather exponential.
- Determine more sampling points to obtain better estimates of the gradients.
- Measure the stepchange close to the influent ($S_O(x=0)$).

Ideal Reactors, Disinfection

1. Fraction of disinfected organisms

The first step is to set up the mass balance for the bacteria.

$$\frac{\partial X_{B,1}}{\partial t} = \frac{Q}{V/6} (X_{B,in} - X_{B,1}) - k_D \cdot X_{B,1} \cdot S_{O_3,1} = 0 \quad (\text{Steady State})$$

Because we are interested in the fraction of organisms, it is possible to divide by the inlet concentration:

$$\frac{\partial x_1}{\partial t} = \frac{Q}{V/6} (1 - x_1) - k_D \cdot x_1 \cdot S_{O_3,1} = 0 \quad (\text{Steady State}) \quad , x_1 = \frac{X_{B,1}}{X_{B,in}}$$

The same can be done for the next five reactors:

$$\frac{\partial x_i}{\partial t} = \frac{Q}{V/6} (x_{i-1} - x_i) - k_D \cdot x_i \cdot S_{O_3,i} = 0 \quad (\text{Steady State}) \quad , x_i = \frac{X_{B,i}}{X_{B,in}}$$

To calculate the fraction of disinfection for each reactor, the concentration of ozone in all the reactors must be calculated:

$S_{O_3,1} = 0.5 \text{ g}_{O_3} \text{ m}^{-3}$ (this is the amount added and no mass balance is required)

For reactors 2 to 6 we write $\frac{\partial S_{O_3,i}}{\partial t} = \frac{Q}{V/6} \cdot (S_{O_3,i-1} - S_{O_3,i}) - k_{O_3} \cdot S_{O_3,i} = 0$ (Steady State)

With these equations we are able to fill the following table:

Reactor	$S_{O_3,i}$ $\text{g}_{O_3}/\text{m}^3$	x_i (= $X_{B,i}/X_{B,in}$)
1	0.5	$7.41 \cdot 10^{-2}$
2	0.429	$6.32 \cdot 10^{-3}$
3	0.367	$6.21 \cdot 10^{-4}$
4	0.315	$7.00 \cdot 10^{-5}$
5	0.270	$9.03 \cdot 10^{-6}$
6	0.231	$1.33 \cdot 10^{-6}$

The total fraction of organisms, that is still alive in the outlet, is $1.33 \cdot 10^{-6}$.

2. Impact of different number of reactors

The code in BM looks as follows:

```
METHOD RK4
STARTTIME = 0
STOPTIME = 1
DT = 0.0001

Vtot = 1000
V = Vtot/n
Q = 10000
kO3 = 10
kD = 1500
n = 6
SO3 = 0.5

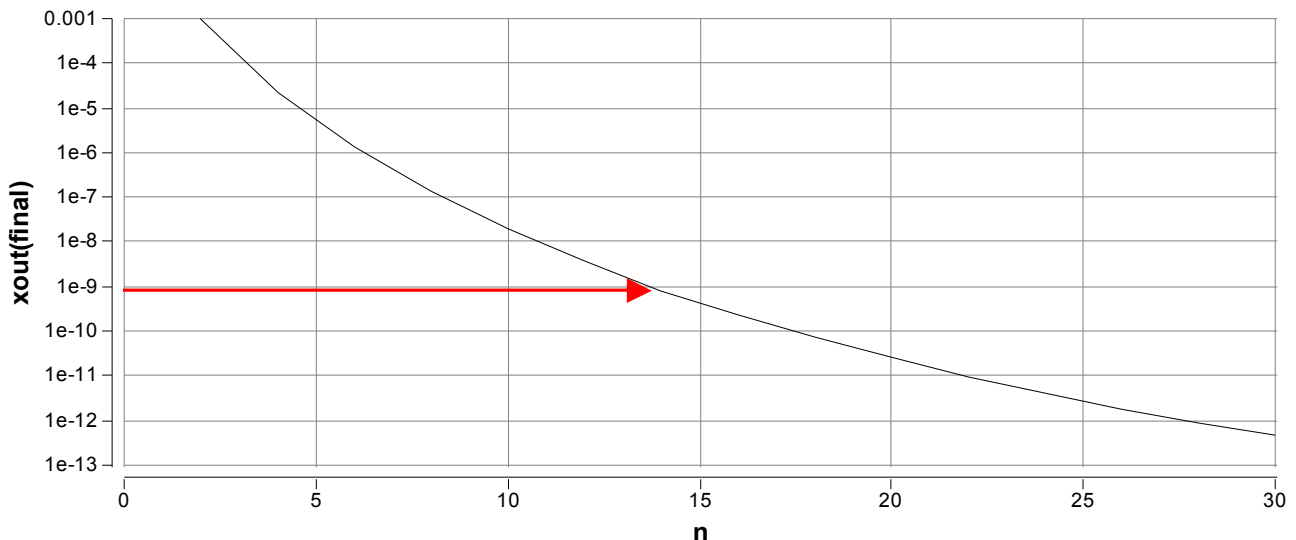
init S[1] = SO3
init S[2..n] = SO3

d/dt (S[1]) = 0
d/dt (S[2..n]) = (Q/V*(S[i-1]-S[i]))-(kO3*S[i])

init x[1..n] = 1 ;x1=X1/Xin and
x2=X2/Xin...
d/dt (x[1]) = (Q/V*(1-x[1])) - (kD*S[1]*x[1])
d/dt (x[2..n]) = (Q/V*(x[i-1]-x[i])) - (kD*S[i]*x[i])

Sout = S[n]
xout = x[n]
```

If you vary the number of reactors from 2 to 30, the efficiency of the disinfection increases with the number of reactors. In the following figure the result is shown by using the function "Parameter Plot". Be aware of the logarithmic scale on the y-axis.



3. Design

The residual concentration of organisms in the effluent falls below the demanded value with a minimum of 14 reactors. If this is not realistic, we could also increase SO3[1] to 0.7. Then 10 reactors would be sufficient.

Ideal Reactors, SBR

1. Development of the concentration of soil during the rinsing process

Some assumptions are made to solve the exercise. The initial value of the mass of soil was chosen as 100 g (=100%). The idea is that we can directly read out of the figure when the required 99% removal is reached.

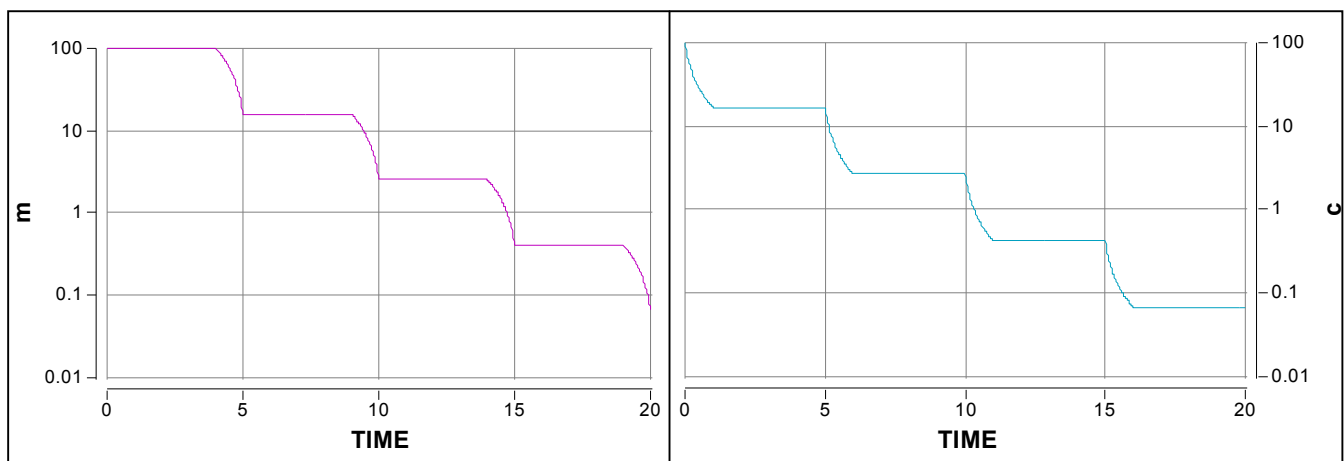


Figure 1: The dynamic behaviour of the mass (left, initial value = 100 g) and the concentration (in g/l) of soil. On the x-axis is the time in minutes.

BM-Code:

```
METHOD RK4
STARTTIME = 0
STOPTIME = 20 ; [min]
DT = 0.02
Q = 5 ; [l/min]
out = IF MOD(TIME, 5) >= 4 THEN 1 else 0
in = IF MOD(TIME, 5) <= 1 THEN 1 else 0
Qout = out * Q
Qin = in * Q
init V = 1
d/dt (V) = Qin - Qout
init m = 100
d/dt (m) = - Qout * c
c = m/V
```

2. Required cycles

Looking at Figure 1 it could be said, that after **3 cycles** the required removal of 99% is reached.

The analytical solution looks as follows.

The concentration of soil during the decanting of 5 liters stays constant. In the first cycle the concentration has the initial value of c_0 . The concentration in the next cycle is lower due to dilution (m_2 : mass of soil in the washing machine in the second cycle; c_1 : the concentration resulting in the second cycle; n : number of required cycles; $c_n = 0.01 \cdot c_0$)

$$c_1 = \frac{m_2}{V_{full}} = \frac{V_{full} \cdot c_0 - V_{dec} \cdot c_0}{V_{full}} \quad , V_{dec} = \frac{5}{6} V_{full}$$

$$= \frac{V_{full} \cdot c_0 \cdot \left(1 - \frac{5}{6}\right)}{V_{full}} = \frac{1}{6} \cdot c_0$$

$$\rightarrow c_n = \left(\frac{1}{6}\right)^n \cdot c_0$$

3. Reversible first-order process during tumbling

To be able to consider the reactions of soil releasing it must be differentiated between the soil within the textiles (xTex) and the soil in the bulk of the water (cL). Therefore two massbalances are needed, whereas for the soil in the bulk of the water it must be considered that the volume changes during a cycle.

BM-Code:

```
METHOD RK4
STARTTIME = 0
STOPTIME = 20 ; [min]
DT = 0.02

;Define In-/Outflow
;=====
Q = 5 ; [l min-1]
out = IF MOD(TIME, 5) >= 4 THEN 1 else 0
in = IF MOD(TIME, 5) <= 1 THEN 1 else 0
Qout = out * Q
Qin = in * Q

;Reaction only during tumbling
;=====
tumbling = if MOD(TIME,5) <= 1 or MOD(TIME,5) >=4 THEN 0 else 1
kforward = 0.5 ; [min-1]
kbackward = 0.5 ; [min-1]
```

```

;Massbalances
;=====
init V      = 1 ; Reactor volume
d/dt (V)   = Qin - Qout

init xTex   = 1 ; soil concentration in the textiles
d/dt(xTex) = if tumbling THEN -kforward*xTex + kbackward*cL else 0

init mL     = 0 ; mass of soil in the bulk of the water
d/dt(mL)   = if tumbling THEN -Qout*cL + kforward*xTex*V - kbackward*cL*V else -Qout*cL

cL          = mL/V ; soil concentration in the bulk
mtot        = cL*xTex ; total mass of soil in the washing maschine

```

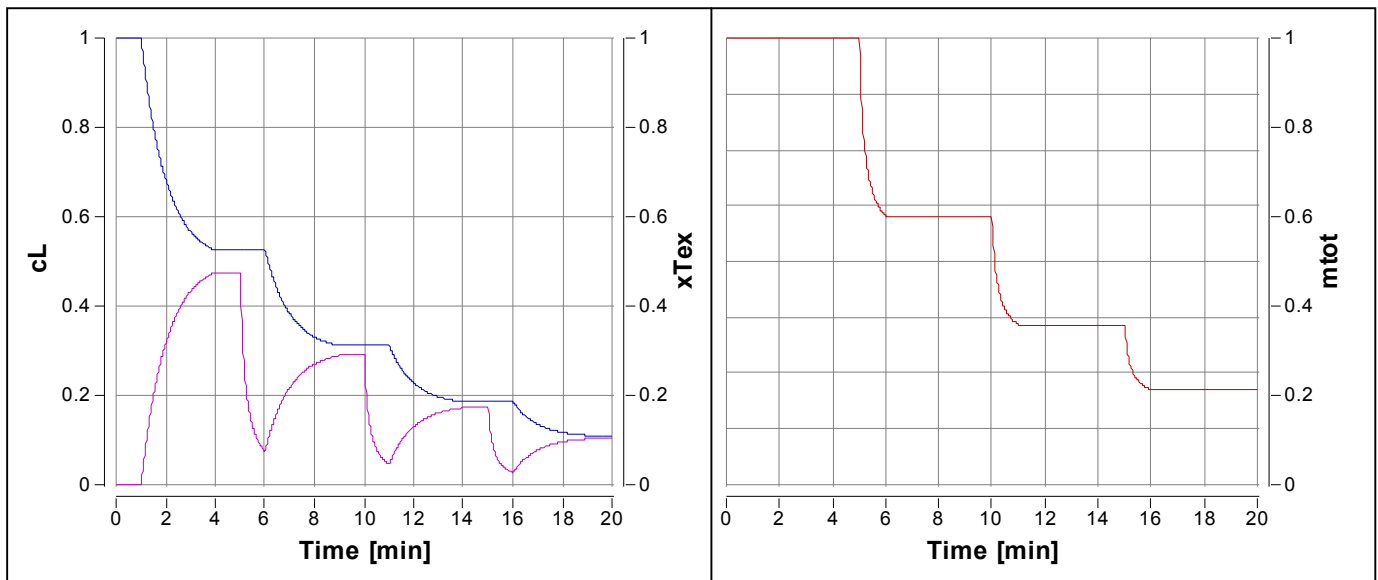


Figure 2: The concentration of soil in the textile (blue) and concentration in the water bulk (pink) are shown in the left part. The total mass in the maschine (red) is shown in the right part.

4. Improvement of rinsing process

In order to save water the tumbling time must be long enough to reach equilibrium. It is useless to tumble longer because no more soil gets in solution. In the BM-code we must therefore define three new parameters (t_{cycle} , t_{fill} , t_{tumbling}). The massbalances from task 3 must be added to the code below.

BM-Code:

```

METHOD RK4
STARTTIME = 0
STOPTIME  = 30 ; [min]
DT        = 0.02

t_cycle   = 5
t_fill    = 1
t_tumbling = t_cycle - t_fill

```

```

;Define In-/Outflow
;=====
Q      = 5          ; [l min-1]
out    = IF MOD(TIME, t_cycle) >= t_tumbling THEN 1 else 0
in     = IF MOD(TIME, t_cycle) <= t_fill THEN 1 else 0
Qout   = out * Q
Qin    = in * Q

;Reaction only during tumbling
;=====
tumbling = if MOD(TIME, t_cycle) <= t_fill or MOD(TIME, t_cycle) >= t_tumbling THEN 0 else 1
kforward = 0.5    ; [min-1]
kbackward = 0.5   ; [min-1]
...
...

```

The influence of the cycle duration may be seen from Figure 3 (3min, 5min and 7min). Now to be able to answer the question whether water will be saved by changing the cycle duration, the amount of water is calculated until a cleaning rate of 99% is reached ($\rightarrow m_{tot} = 0.01$). For a cycle duration of 3min 15 cycles are needed and in each cycle 5 l of water are added, in total 75 l is needed. For 5min duration 10 cycles are needed ($\rightarrow Q_{tot} = 50$ l) and for 7min duration also 10 cycles ($Q_{tot} = 50$ l). The reason for the stagnation is that with 5min cycles the equilibrium concentration is nearly reached, so longer cycles are not useful.

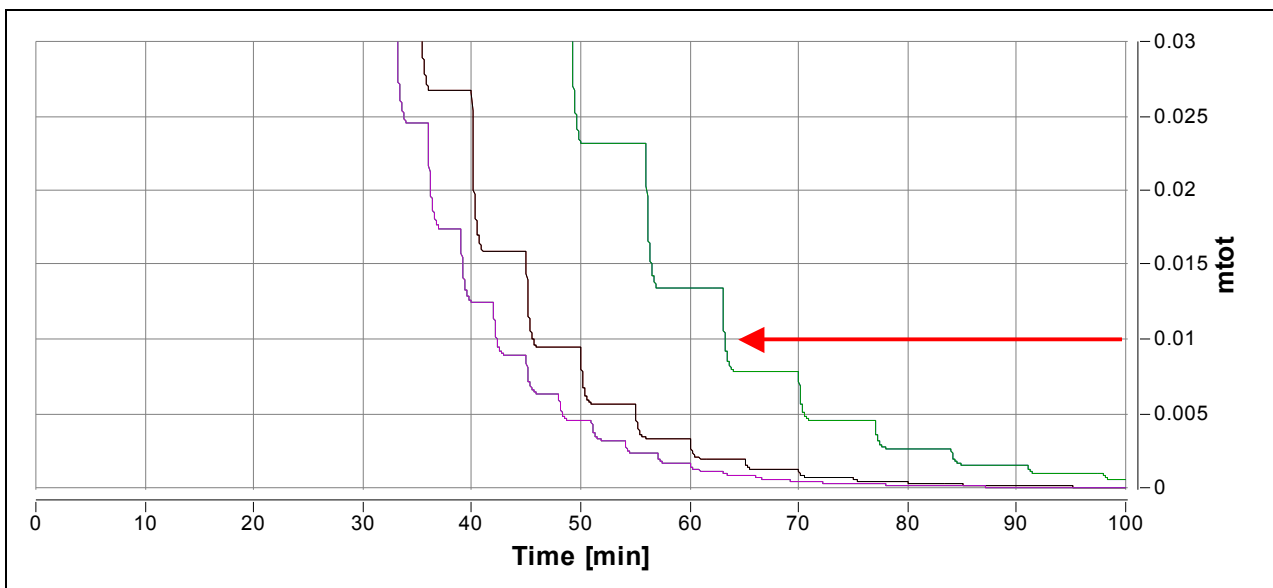


Figure 3: The influence of cycle duration: $t_{cycle} = 5$ min (black), $t_{cycle} = 3$ min (pink), $t_{cycle} = 7$ min (green). All other parameters stayed unchanged from task 3.

Another possibility is to reduce the amount of water per cycle. In Figure 4 the results of three different Q (2 l per cycle, 5 l per cycle and 8 l per cycle) are presented. Again for each condition the total amount of water is calculated until 99% removal is reached. For 5 l the amount was already calculated before ($Q_{tot} = 50$ l). For 8 l per cycle in total 80 l are needed and for 2 l only 26 l are necessary. There is a clear improvement with less water per cycle, but 13 cycles will be necessary.

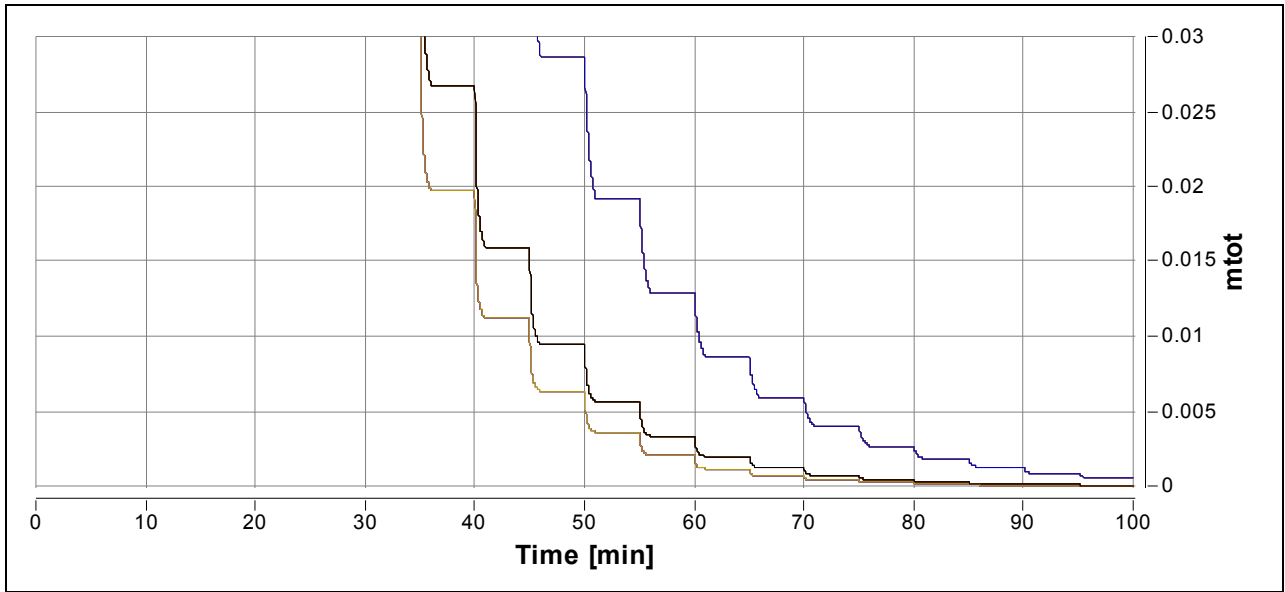


Figure 4: Influence of amount of water per cycle. $Q = 5$ l/min (black), $Q = 8$ l/min (yellow), $Q = 2$ l/min (blue). All other parameters stayed unchanged from task 3.

Residence Time Distribution – Cascade of CSTRs

1. Flow rate Q:

Idea: The total mass of the tracer in the outflow must be equal to the amount of added tracer substance ($M_{T,add}$) in the inflow. This is shown in the equation below, it is assumed that the flow rate (Q) is constant:

$$M_{T,add} = \int_{t=0}^{\infty} Q \cdot c_{T,out} \cdot dt \quad c_{T,out} = \text{outflow-concentration of tracer} \quad (1)$$

$$= Q \cdot \int_{t=0}^{\infty} c_{T,out} \cdot dt \quad Q = \text{constant} \quad (2)$$

The integral in equation 2 can not be calculated exactly. But the area below the curve in Fig. 16.3 (in the book *Systems Analysis for Water Technology*, Gujer (2008)) expresses the result of the integral. With a rough optical estimation (approximation of the area by a rectangle) the area can be approximated as $\sim 9 \text{ g h m}^{-3}$.

$$Q = \frac{M_{T,add}}{\int_{t=0}^{\infty} c_{T,out} \cdot dt} \quad (3)$$

$$= \frac{10'000 \text{ g}}{9 \text{ g h m}^{-3}} = 1'111 \text{ m}^3 \text{ h}^{-1}$$

2. Volume of the reactor

The mean hydraulic residence time (τ_m) is a function of the volume and the flow rate (equation 4), which was calculated in task 1. The mean hydraulic residence time can be approximated by separating the area below the curve in Fig. 16.3 into two parts of equal area, $\tau_m \approx 0.7 \text{ h}$.

$$\tau_m = \frac{V}{Q} \quad (4)$$

$$V = Q \cdot \tau_m = 777 \text{ m}^3$$

3. Number of reactors in series

The number of reactors has an influence on the “distribution” of the outflow concentration. This is expressed in equation 5, where the number of reactors (n) is a function of the mean hydraulic residence time and the variance σ^2 of the curve.

$$n = \frac{\tau_m^2}{\sigma^2} \quad (5)$$

To estimate the variance optically it is easier to estimate first the double size of the standard deviation (2σ). It is approximated that $2\sigma = 0.5$ h. If the standard deviation is inserted in equation 5, the number of reactors can be calculated (equation 6):

$$n = \frac{(0.7\text{h})^2}{(0.25\text{h})^2} \cong 8 \quad (6)$$

Remark:

To identify the parameters more detailed, a BM-code can be written and by trial-and-error the best fit can be found. As start values it is recommended to use the calculated values in the tasks 1 and 2.

BM-Code:

```
METHOD RK4
STARTTIME = -1
STOPTIME = 10 ; [h]
DT = 0.002
M = 10000 ; [g]
Cin = PULSE(M/Q, 0,1000)
Q = 1250 ; [m3 h-1]
Vtot = 875 ; [m3] , Vtot = 0.7*Q
V = V/n
n = 12
init C[1..n] = 0
d/dt (C[1]) = Q/V * (Cin - C[1])
d/dt (C[2..n]) = Q/V * (C[i-1] - C[i])
cout = C[n]
```


RTD – Activated Sludge Tank

1. Develop a model:

Firstly the activated sludge tank must be discretized as a cascade of CSTRs. In this approach the flow scheme in Figure 1 is used. Obviously there are several other solutions possible. In a second step the mass balance equations for all the reactors must be set up and implemented in Berkeley Madonna.

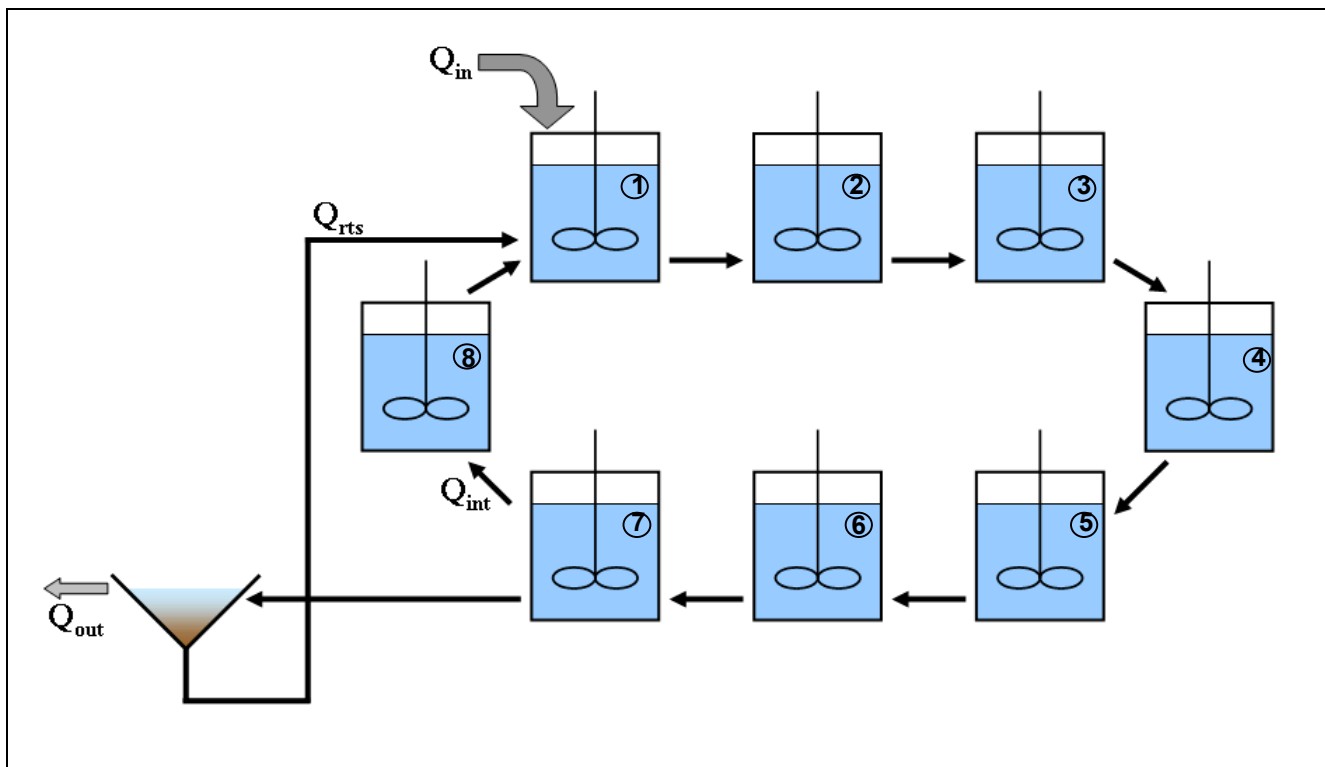


Figure 1: Flow scheme of the activated sludge reactor with high internal recirculation

BM-Code:

```
METHOD RK4

STARTTIME = -0.1           ; time in days
STOPTIME=5
DT = 1E-4

M = 10000                  ; mass of tracer in g
Cin = pulse(M/Q,0,1000)   ; input of tracer
```

```

Q = 10000           ; Influent m3 d-1
R = 10000           ; returnsludge m3 d-1
Qc = 120000         ; internal recirculation, m3 d-1
Vtot = 5000         ; m3

n = 8               ; number of reactors
V = Vtot / n        ; volume of one reactor m3
tR = 1/24           ; delay of returnsludge d
CR = delay(C[n-1],tR) ; conc. in return sludge g m-3

init C[1..n] = 0
d/dt(C[1]) = (Q*Cin+R*CR+Qc*C[n]-(Q+R+Qc)*C[1])/V
d/dt(C[2..n-1]) = (Q+R+Qc)*(C[i-1]-C[i])/V
d/dt(C[n]) = Qc*(C[n-1]-C[n])/V

Cout = C[n-1]

```

2. Hydraulic residence time distribution

To determine the hydraulic residence time of the reactor two lines of code need to be added to the above model:

```

init tauC = 0
d/dt(tauC) = time*Q*Cout/M ; mean residence time (eqn. 7.5)

```

In addition to the cascade the residence time distribution for a single CSTR must be modelled. Therefore the BM-code below is needed in addition to the code that was used for task 1.

```

{ single CSTR with delayed recycle }
init S = 0
d/dt(S) = (Q*Cin+R*delay(S,tR) - (Q+R)*S)/Vtot
init tauS = 0
d/dt(tauS) = time*Q*S/M ; mean residence time (eqn. 7.5)

```

The mean residence time of the reactor exceeds $V_{tot}/Q = 0.5$ d because the delay of the return sludge includes some volume of the secondary clarifier ($R \cdot \text{delay} = 10000/24 = 417$ m³). This results in $5417/10000 = .54$ d. The residence time distributions of the two reactor models differ only in the very first period until the reactor contents are mixed by the internal recirculation.

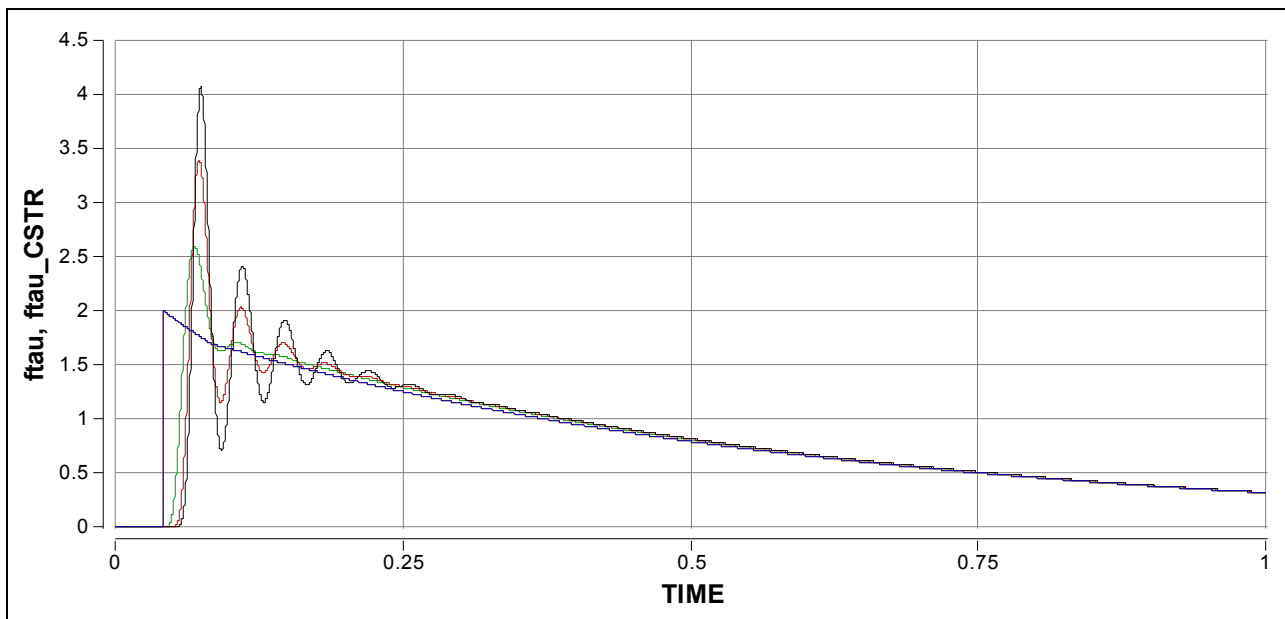


Figure 2: RTD: single CSTR (blue), cascade n=8 (green), n=16 (red) and n=24 (black).

3. Mean hydraulic residence time

In a first step the mean hydraulic residence time is calculated by the general equation (1). This can be subsequently compared with the simulated mean hydraulic residence time (end value of τ in BM-code of task 2).

$$\tau_m = \frac{V}{Q} \quad (1)$$

$$= \frac{5'000 \text{ m}^3}{10'000 \text{ m}^3 \text{ d}^{-1}} = 0.5 \text{ d} = 12 \text{ h}$$

The simulated τ_m is $\sim 14\text{h}$. The reason for the difference is the additional retention of the return sludge in the secondary clarifier.

4. Performance of the two models

The mass balances must be adapted to be able to describe a degradation. Additionally the inflow concentration was assumed to be 1 (100%), this way it is possible to determine the performance of the two linear models directly based on the outflow concentrations.

BM-code:

```
METHOD RK4

STARTTIME = -0.1 ; time in days
STOPTIME=5
DT = 1E-4

Cin =1 ; inflow concentration for 1st order reaction
Q = 10000 ; Influent m3 d-1
R = 10000 ; returnsludge m3 d-1
Qc = 120000 ; internal recirculation, m3 d-1
Vtot = 5000 ; m3
```

```

n = 8                ; number of reactors
V = Vtot / n        ; volume of one reactor m3
tR = 1/24           ; delay of returnsludge d
CR = delay(C[n-1],tR) ; conc. in return sludge g m-3

k = 24              ; rate constant d-1

init C[1..n] = 0
d/dt(C[1]) = (Q*Cin+R*CR+Qc*C[n]-(Q+R+Qc)*C[1])/V+rC[1]
d/dt(C[2..n-1]) = (Q+R+Qc)*(C[i-1]-C[i])/V+rC[i]
d/dt(C[n]) = Qc*(C[n-1]-C[n])/V+rC[i]

rC[1..n] = -k*C[i]
Cout = C[n-1]

{ single CSTR with delayed recycle }
init S = 0
d/dt(S) = (Q*Cin+R*delay(S,tR) - (Q+R)*S)/Vtot - k*S

```

The outflow concentration expresses directly the percentage of substance in the outflow. Therefore the performance P is defined as follows:

$$P = 1 - c_{out}$$

With this equation results a performance of around 94% for the model of a cascade with 8 CSTRs and 92% for the model of a single CSTR. The small difference stems from the small trend towards a more plug flow like character of the cascade.

RTD, Flow rate and Dispersion in a Sewer

1. Flow rate Q in the sewer

It is assumed that the sewer can be modelled with a turbulent plug-flow reactor, closed for turbulence. Further it is assumed, that the background concentration of the tracer that was used, was zero ($C_{A,0} = 0$) and the flow rate Q is constant.

In an experiment with pulse addition of a tracer, the following applies:

$$E_A = \int_0^{\infty} Q * C_A * dt = Q * \int_0^{\infty} C_A * dt \quad \text{if } Q = \text{const.}$$

We can see in Fig. 16.5 that after 1800 seconds, the integrated effluent concentration has reached a value of about 9.2 g*s/m^3 . This value corresponds to the total tracer mass ($E_A = 1 \text{ g}$) divided by the flow rate Q:

$$\int_0^{1800 \text{ s}} C_A * dt = 9.2 \frac{\text{g} * \text{s}}{\text{m}^3} = \frac{E_A}{Q} \rightarrow Q = \frac{1 \text{ g}}{9.2 \frac{\text{g} * \text{s}}{\text{m}^3}} = 0.108 \frac{\text{m}^3}{\text{s}}$$

2. Mean flow velocity in the sewer

According to Fig. 16.5, the mean hydraulic residence time θ_h is assumed to be about $1090 \text{ s} = 0.3 \text{ h}$.

$$\theta_h = \frac{L}{u} \rightarrow u = \frac{L}{\theta_h} = \frac{1500 \text{ m}}{1090 \text{ s}} = 1.38 \frac{\text{m}}{\text{s}}$$

3. Dispersion coefficient in the sewer

Equation 7.37 relates the mean and variance of the hydraulic residence time with the turbulence number N_T :

$$\frac{\sigma^2}{\tau_m^2} = \frac{1}{n} = 2 * N_T - 2 * N_T^2 * \left(1 - \exp\left(-\frac{1}{N_T}\right)\right)$$

$$\text{With } \sigma \approx 110 \text{ s} \rightarrow N_T = 0.005$$

The dispersion coefficient in the sewer is thus:

$$D_T = N_T * u * L = 0.005 * 1.38 \frac{\text{m}}{\text{s}} * 1500 \text{ m} = 10.60 \frac{\text{m}^2}{\text{s}}$$

Modeling a Sewer

1. Sewer modelled as a cascade of CSTRs

Given a particular sewer, say with a length of $L = 1000$ m and a flow velocity of $u = 1$ m/s (typical value in a sewer), the turbulence number N_T can be estimated with the help of Eq. 7.40:

$$N_T = \frac{D_T}{u * L} = \frac{0.15 \frac{m^2}{s}}{1 \frac{m}{s} * 1000 m} = 0.00015$$

Figure 7.19 relates N_T and n (number of required CSTRs in the cascade) by the relationship $2 * N_T = 1/n$. Together with the above equation, n and the specific sewer length per reactor, L/n can be calculated:

$$2 * N_T = \frac{1}{n} \rightarrow n = \frac{1}{2 * N_T} = \frac{1}{2 * 0.00015} = 3333.3$$

$$2 * \frac{D_T}{u * L} = \frac{1}{n} \rightarrow \frac{L}{n} = 2 * \frac{D_T}{u} = 2 * \frac{0.15 \frac{m^2}{s}}{1 \frac{m}{s}} = 0.30 m$$

The total number of CSTRs in series needed to model this given sewer is 3333 ($= n$). This is a large number and approximates true plug flow. It can be seen that the specific sewer length is only dependent on u and D_T . Each CSTR would model the equivalent of 0.3 m sewer.

Rieckermann et al. (2005) obtained their value for D_T in a straight sewer with a flow velocity of approximately $u = 0.5$ m/s. With this value we would obtain $n = 1667$. But this would only increase the length of each element to 0.67 m.

A simulation of a residence time distribution with $n = 3333$ and $u = 1$ m/s is given below.

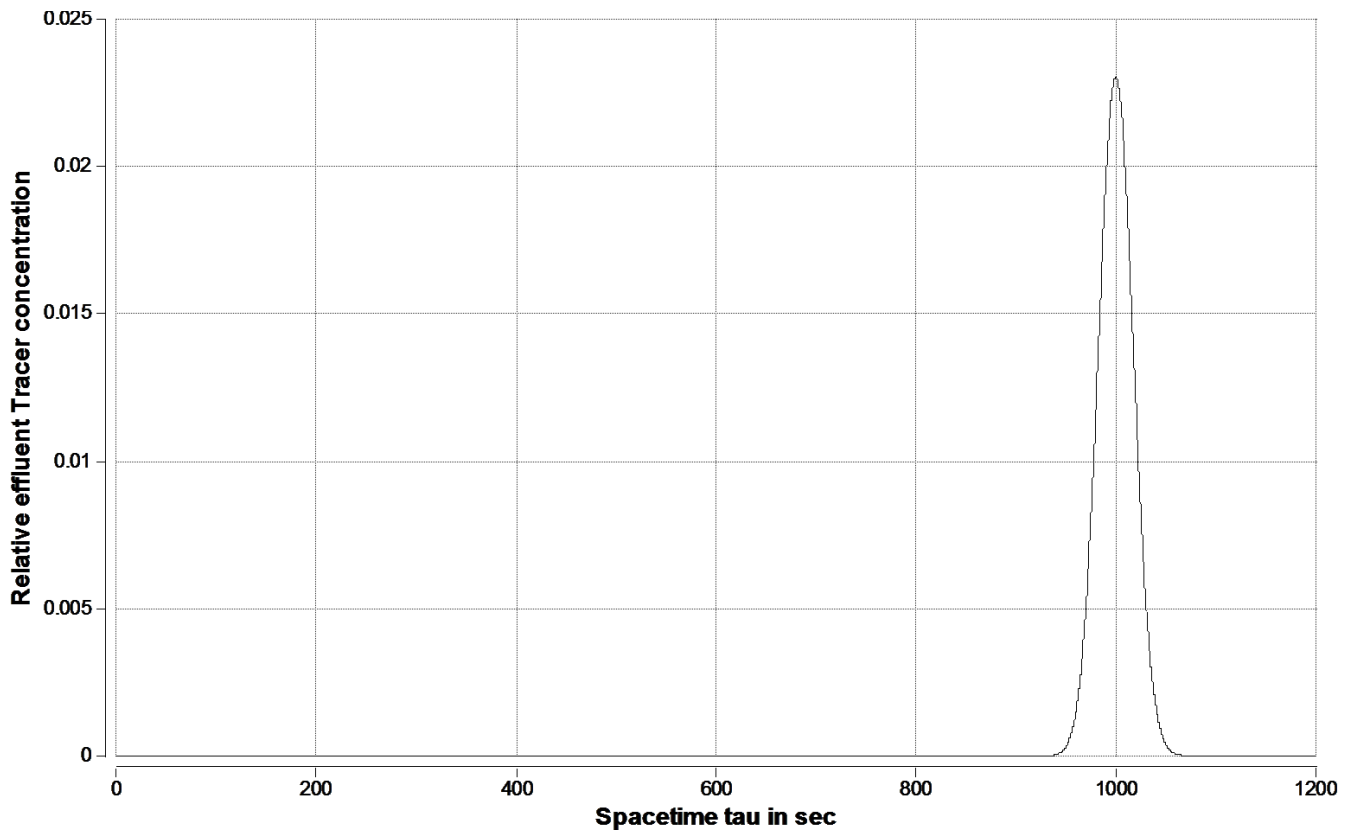


Figure 1: Residence time distribution for a plug-flow reactor with $n = 3333$ and $u = 1$ m/s.

2. Sewer modelled as a turbulent plug-flow reactor

Numeric models of a turbulent plug-flow reactor will always have a higher n than the cascade of CSTRs since we introduce additional backmixing. Additional backmixing would only serve to increase N_T which would then have to be compensated with an increased number of elements in series. Therefore, if 1000 m of sewer already require 3333 CSTRs in series, we would use $R = 0$ and keep the cascade as a limiting case. The numeric model for the turbulent plug-flow reactor would thus be identical to the cascade of CSTRs.

Alternatively, the analytical equations for the turbulent plug-flow model can easily be solved for steady state (under the assumption of a reactor closed for turbulence).

RTD, Disinfection Reactor

1. RTD of a disinfection reactor for 2, 6 and 30 reactors in series.

The disinfection reactor from problem 16.9 is modeled as a cascade of CSTRs.

A visual comparison of the residence time distributions $f(\tau)$ for a cascade of 2 CSTRs (green), 6 CSTRs (red) and 30 CSTRs (black) is given in Figure 1:

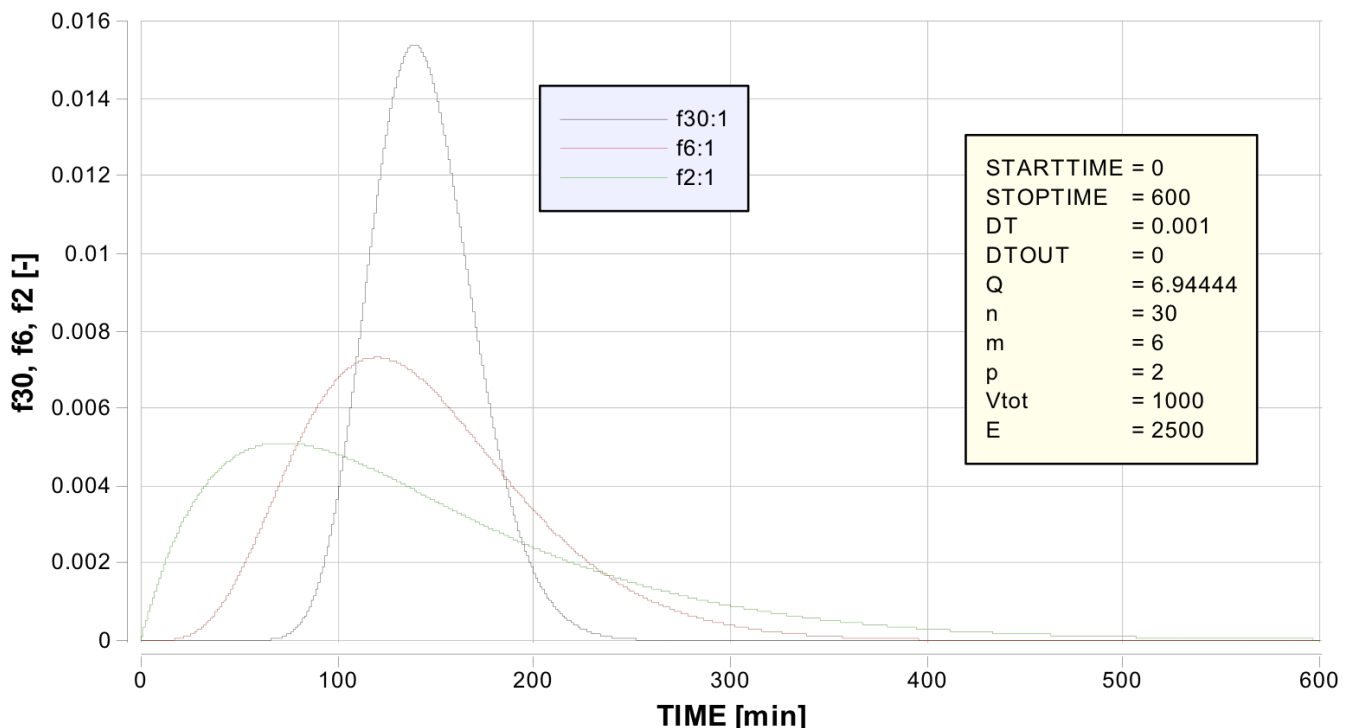


Figure 1: Residence time distributions $f(\tau)$ for a cascade of 2, 6 and 30 CSTRs in series.

The cascade of 30 reactors shows a residence time distribution (RTD) close to a normal distribution around the mean value τ_m , 144 min. The RTD for 2 reactors in series is left skewed, and the one for 6 reactors in series is somewhere in between.

It can be concluded that the higher the number of reactors in series (n) we model, the more the residence time distribution approaches the shape of a normal distribution. This means also that the distribution gets more and more narrow and the variance decreases considerably (see Table 1).

Table 1: Summary of RTD characteristics for the three reactor configurations.

Reactor configuration	Mean hydraulic residence time τ_m [min]	Variance σ^2 [min ²]
n = 2	144.001	10'368.0
n = 6	144.001	3456.0
n = 30	144.001	691.2

RTD, Additivity of τ_m and σ^2

For reactors that are closed to turbulence, which means that advection dominates dispersion in the influent and effluent, the tracer concentration in the effluent can be calculated with the help of a convolution integral. A convolution integral has mathematical properties that lead to the fact, that the expected value τ_m and the variance σ^2 of the residence time are additive. (see chapter 7.3)

For the derivation of the equations 7.25 and 7.26 a cascade of n reactors is assumed. All reactors have the same volume V_i , so the total Volume equals $V_{tot} = \sum_{i=1}^n V_i = n \cdot V_i$.

The expected value of the residence time of a single reactor is calculated by $\tau_{m,i} = \frac{V_i}{Q} = \theta_{h,i}$ (see equation 7.22). The equation for the variance of a single reactor is $\sigma_{i,i}^2 = \theta_{h,i}^2$ (see equation 7.23). According to these assumptions, the properties of a cascade of reactors can be derived as follows:

$$\tau_{m,tot} = \theta_{tot} = \sum_{i=1}^n \theta_i = n \cdot \theta_i = \sum_{i=1}^n \frac{V_i}{Q} = \frac{1}{Q} \cdot \sum_{i=1}^n V_i = \frac{V_{tot}}{Q} = \theta_h$$

$$\sigma_{tot}^2 = \sum_{i=1}^n \sigma_i^2 = \sum_{i=1}^n \theta_i^2 = n \cdot \left(\frac{V_i}{Q}\right)^2 = n \cdot \left(\frac{V_{tot}}{n \cdot Q}\right)^2 = \frac{n}{n^2} \cdot \left(\frac{V_{tot}}{Q}\right)^2 = \frac{\theta_h^2}{n}$$

RTD, Turbulent Plug-Flow Reactor

1. Turbulence number N_T

The turbulence number N_T is calculated according to Equation 7.32:

$$u = \frac{Q}{A} = \frac{500 \frac{m^3}{h}}{20 m^2} = 25 \frac{m}{h}$$

$$N_T = \frac{D_T}{u * L} = \frac{300 \frac{m^2}{h}}{25 \frac{m}{h} * 50 m} = 0.240$$

2. Model A: Cascade of CSTRs

The following equation (7.37) relates the number of CSTRs in a cascade (n) with the turbulence number N_T :

$$\frac{\sigma^2}{\tau_m^2} = \frac{1}{n} = 2 * N_T - 2 * N_T^2 * \left(1 - \exp\left(-\frac{1}{N_T}\right)\right)$$

With the above value of $N_T = 0.240$, the equation can be solved for n :

→ SOLVER: $n = 2.73 \approx 3$

The main parameter of a cascade of CSTRs model is the integer n . With small n we cannot very accurately approximate the behaviour of the system to be modelled.

3. Model B: 30 CSTRs in series with backmixing rate R

For numeric simulation, the turbulent PFR is discretized in n discretization steps, which are represented as single CSTRs in series. With the internal back mixing rate R between the CSTRs, we can model the transport of material by turbulence or dispersion. But we also have to consider the additional dispersion induced by the cascade, which has to be subtracted from the total turbulence number $N_{T,tot}$ found in subtask 2.

Cascade:
$$\frac{1}{n} = 2 * N_{T,C} - 2 * N_{T,C}^2 * \left(1 - \exp\left(-\frac{1}{N_{T,C}}\right)\right) \rightarrow N_{T,C}(n = 30) = 0.0170$$

Back mixing:
$$N_{T,R} = N_{T,tot} - N_{T,C} = 0.240 - 0.0170 = 0.223$$

$$R = N_{T,R} * n * Q = 0.223 * 30 * 500 \frac{m^3}{h} = 3345.7 \frac{m^3}{h}$$

4. Comparison of performance of model A and B for a first order process with decay rate $k = 2 \text{ h}^{-1}$.

Choosing an influent concentration of 100 g/m^3 , model A achieves an effluent concentration of 7.9 g/m^3 and a removal efficiency of $(1 - S_{\text{eff}}/S_{\text{in}}) \cdot 100\% = 92.1 \%$ (see Figure 1).

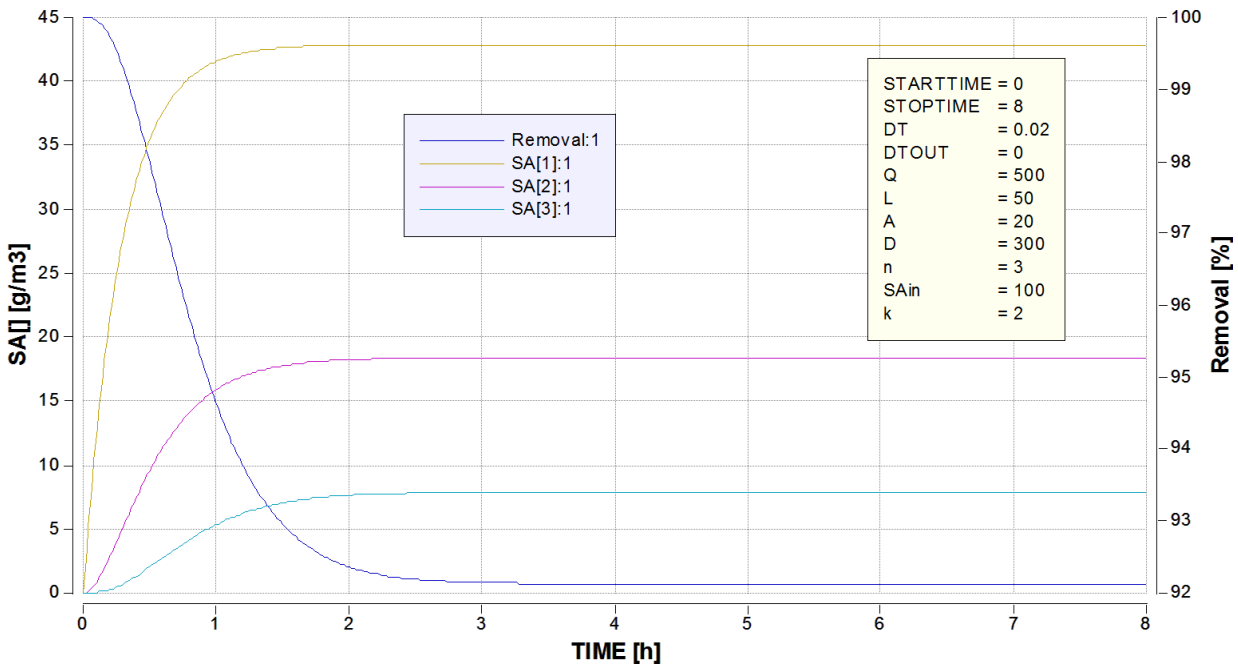


Figure 1: Effluent concentration and removal efficiency of model A (Cascade of 3 CSTRs).

Model B achieves an effluent concentration of 7.1 g/m^3 and a removal efficiency of $(1 - S_{\text{eff}}/S_{\text{in}}) \cdot 100\% = 92.9 \%$ (see Figure 2). In terms of both absolute and relative performance, model B is better, the difference to model A is small though.

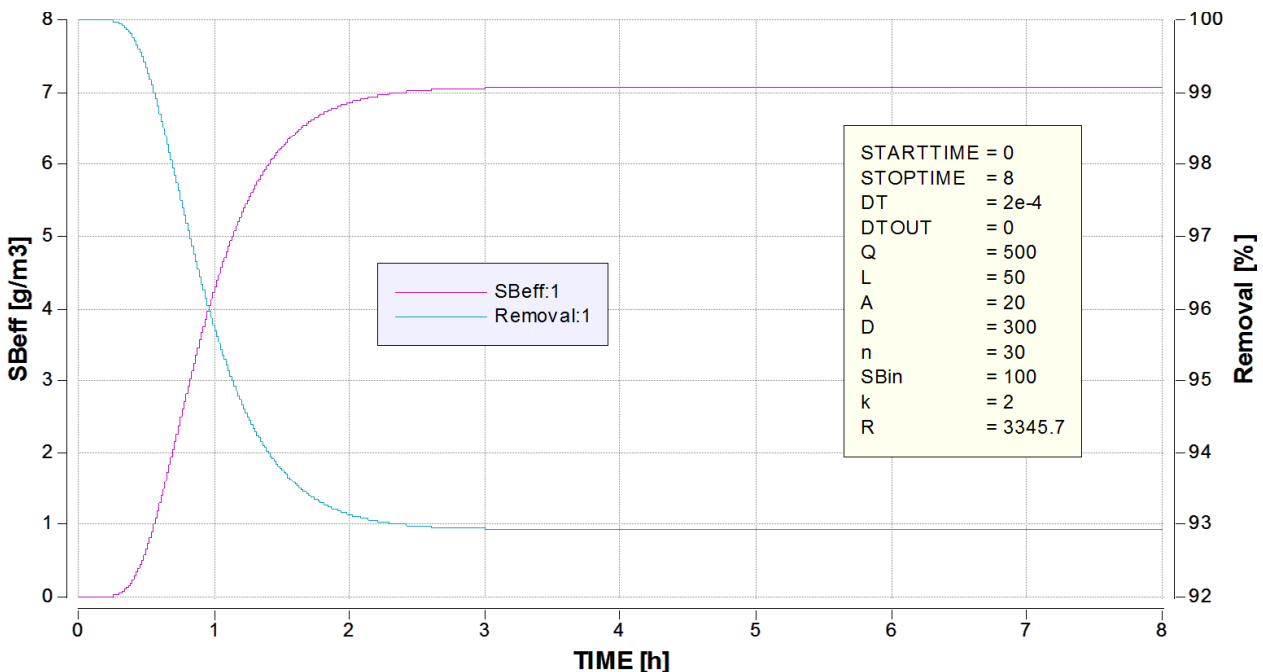


Figure 2: Effluent concentration and removal efficiency of model B (30 CSTRs in series with back mixing rate $R = 3345.7 \text{ m}^3/\text{h}$).

5. Model C: Numeric solution of the mass balance equation for the turbulent plug-flow reactor.

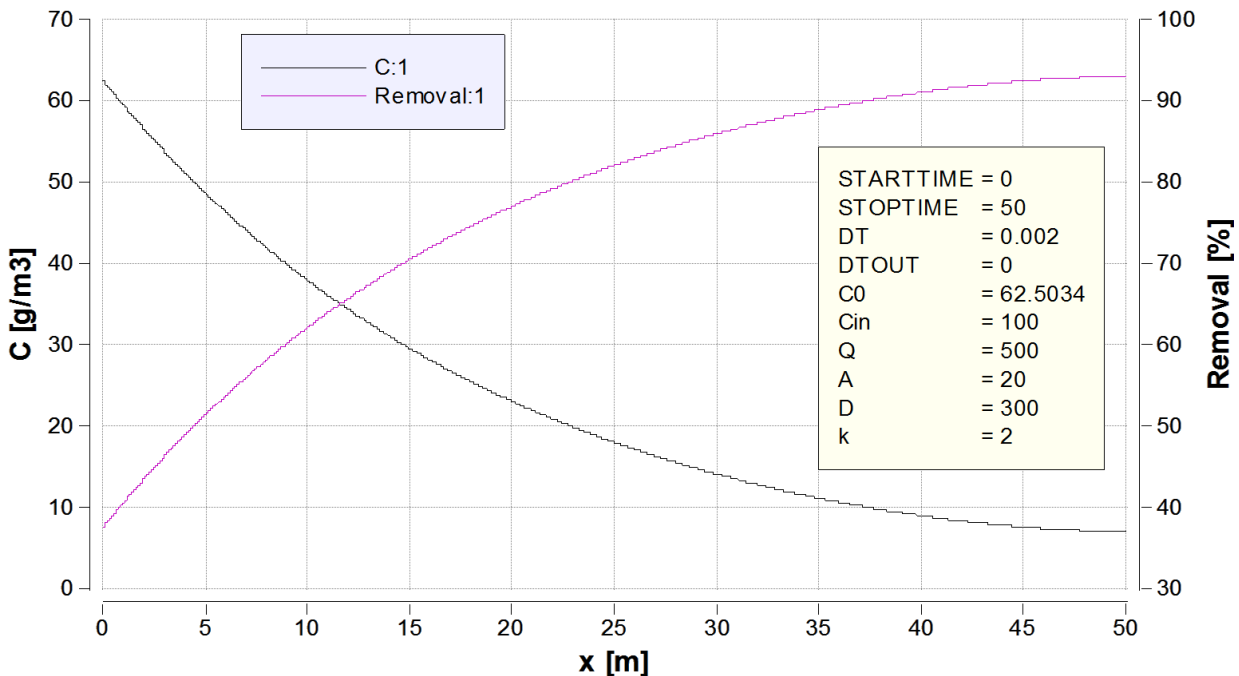


Figure 3: Effluent concentration and removal efficiency of model C (numeric solution of mass balance for turbulent PFR).

If we assume again a decay rate k of 2 h^{-1} , model C achieves an effluent concentration of 7.1 g/m^3 and a removal efficiency of $(1 - C_{\text{eff}}/C_{\text{in}}) \cdot 100\% = 92.9\%$ (see Figure 3).

It is important to note that the results of model C are strongly dependent on the choice of the timestep DT and the accuracy of the iteration (see Model > Modules > Boundary Value ODE > Tolerance). The results in Figure 3 were attained with a tolerance of $1 \cdot 10^{-5}$.

A comparison of the performance of the two discretized models A and B with the numeric solution of the mass balance equation for the turbulent plug-flow reactor is summarized in Table 1. It can be concluded that model B is a very good approach to model a turbulent PFR, as it reproduces the same results as model C does. This is due to a high number of reactors in series ($n = 30$) and the back mixing R . However, the performance of model A is worse compared to model C.

Table 1: Summary of the performance of the three models.

Model	Effluent concentration [g/m ³]	Removal efficiency [%]
A: Cascade of 3 CSTRs	7.9	92.2
B: 30 CSTRs in series with back mixing	7.1	92.9
C: Numeric solution of turbulent PFR mass balance equation	7.1	92.9

6. Comparison of the hydraulic residence time distributions (RTD) of models A and B (discretized).

The calculation of the hydraulic residence time distribution for both models (see Figure 4) allows to determine the mean hydraulic residence time (τ_m) and the variance of the residence time (σ^2):

Model A: $\tau_m = 2.00$ h
 $\sigma^2 = 1.33$ h²

Model B: $\tau_m = 2.00$ h
 $\sigma^2 = 1.47$ h²

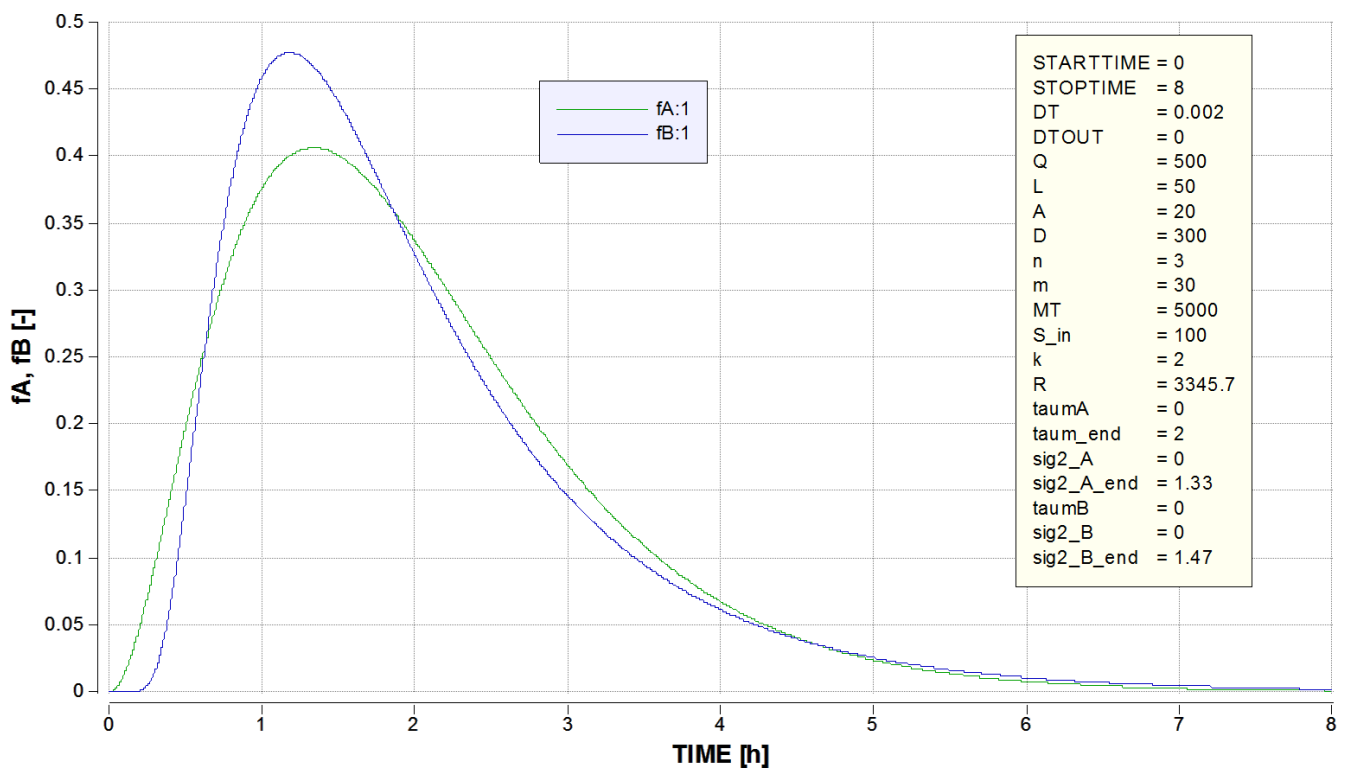


Figure 4: Residence time distribution $f_A(\tau)$ of model A (Cascade of 3 CSTRs) and $f_B(\tau)$ of model B (30 CSTRs in series with back mixing rate $R = 3345.7$ m³/h).

Model B shows a higher variance of the system than model A, since model B considers turbulence between the discrete compartments by including the back mixing rate R . In comparison to model A, the RTD of model B is thinner and has a higher peak, additionally the distribution is more left skewed.

Heterogeneous Systems: Filtration

1. Model for the removal of TSS over the depth of the filter with time

This problem is about developing a model over the time t for a rapid sand filter. Given is, that the concentration of particles C develops over the depth x according to the following equation:

$$\frac{\partial C}{\partial x} = -\lambda * C \quad \text{with} \quad \lambda = \lambda_0 + a_1 * \sigma - \frac{a_2 * \sigma^2}{\sigma_{max} - \sigma}$$

It can be seen that the mass balance of C depends on σ , the accumulated solids in the filter. σ itself changes as well with filter depth and depends on the concentration of particles in the water (C). So it is necessary to develop two mass balances for C and σ , respectively, which are coupled.

Accumulation of solids on the filter

Mass balance:

$$\begin{aligned} & [\text{Rate of gain of particles accumulated in the filter}] \\ & = [\text{Rate of loss of particles from the flowing water}] \end{aligned}$$

$$\text{Discretized: } A * \Delta x * \frac{\partial \sigma}{\partial t} = Q * C(x) - Q * C(x + \Delta x)$$

$$\frac{\partial \sigma}{\partial t} = -\frac{Q}{A} * \frac{(C(x + \Delta x) - C(x))}{\Delta x} = -v_F * \frac{\partial C}{\partial x}$$

$$\text{With } \frac{\partial C}{\partial x} = -\lambda * C: \quad \frac{\partial \sigma}{\partial t} = v_F * \lambda * C$$

$$\rightarrow \frac{\partial \sigma_i}{\partial t} = v_F * \lambda * C_i = v_F * \left(\lambda_0 + a_1 * \sigma_i - \frac{a_2 * \sigma_i^2}{\sigma_{max} - \sigma_i} \right) * C_i$$

σ : accumulated solids in the filter [gTSS/m³_{Filterbed}]

C : TSS concentration in the water [gTSS/m³]

A : cross-section of filter bed [m²]

Δx : discretization step [m]

x : filter depth [m]

ε : porosity [-]

Q : flow rate through filter [m³/h]

v_F : filtration rate [m³/(m²_{Filterbed}*h)]

λ : filtration coefficient [m⁻¹]

$\lambda_0, a_1, a_2, \sigma_{max}, k, a_3$: parameters as indicated in exercise description

Concentration of TSS in the water

In order to model the change of C over the depth x, the filter depth is discretized and is modelled as a cascade of CSTRs.

Mass balance:

$$[Accumulation] = [Influent] - [Effluent] - [Loss]$$

$$\text{Discretized: } A * \Delta x * \varepsilon * \frac{\partial C}{\partial t} = Q * C(x) - Q * C(x + \Delta x) - \frac{\partial \sigma}{\partial t} * A * \Delta x$$

$$\text{Cascade of CSTRs: } \frac{\partial C_i}{\partial t} = \frac{Q}{A * \varepsilon} * \frac{1}{\Delta x} * (C_{i-1} - C_i) - \frac{\partial \sigma}{\partial t} * \frac{1}{\varepsilon}$$

$$\text{With } \Delta x = \frac{L}{n}: \frac{\partial C_i}{\partial t} = \frac{v_F}{\varepsilon} * \frac{n}{L} * (C_{i-1} - C_i) - \frac{v_F}{\varepsilon} * \lambda * C_i$$

ε : porosity [$\text{m}^3_{\text{Water}}/\text{m}^3_{\text{Filterbed}}$]

L: total filter depth [m]

n: number of CSTRs in series [-]

2. Prediction of the head loss

What is given is the head loss H depending on the filter depth x and the accumulated solids σ :

$$\frac{\partial H}{\partial x} = k * \left(\frac{\sigma_{max}}{\sigma_{max} - \sigma} \right)^{a_3}$$

$$\text{With } \partial x = \frac{L}{n} \rightarrow \Delta H_i = \frac{L}{n} * k * \left(\frac{\sigma_{max}}{\sigma_{max} - \sigma_i} \right)^{a_3}$$

It should be noted that the total filter depth L is meant here, so unlike the increase of the concentration in the water and the accumulated solids along the flowing water, H is constant for a certain filter depth.

3. Maximal allowable head loss, backwashing, development over time

Assumptions: porosity ε : 0.4 (typical value for coarse sand)
cross-section A: 50 m^2

Limiting head (maximal allowable head loss): 3 m (given)

Time until limiting head is reached: $t_{HL}(H=3) = 36.8$ h (see Figure 1)

Amount of accumulated solids at that time: $M_{\sigma}(t_{HL}) = 273'985\text{gTSS}$ (see Figure 1)

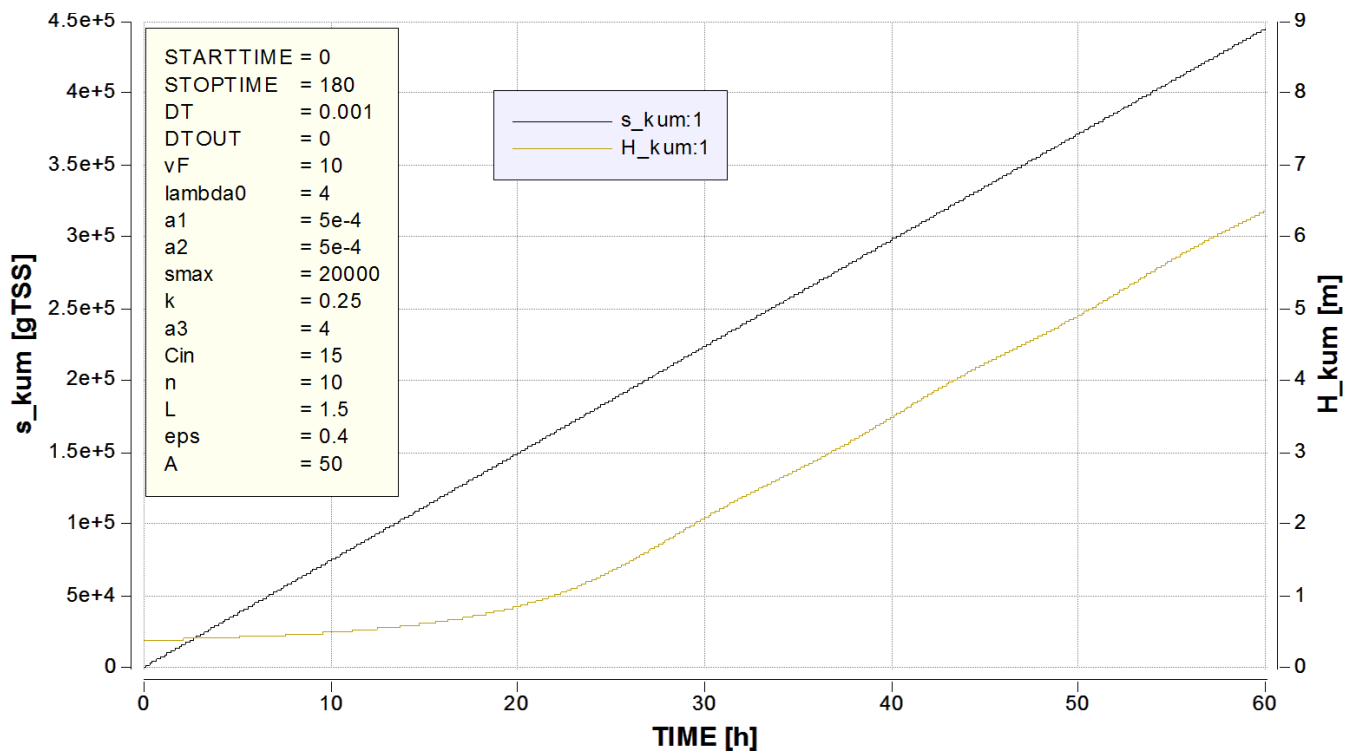


Figure 1: Development of the total mass of accumulated solids and head loss over time.

So the filter would have to be backwashed at least every 36.8 h.

Development over time

It can be seen in Figure 2 that after about 60 h (2.5 days, $t_{\text{Breakthrough}}$), the TSS effluent concentration C_{out} starts to rise, which means that the pollutants will break through the filter. In the end, if the filter was not backwashed, C_{out} would reach the value of the influent concentration, 15 gTSS/m³.

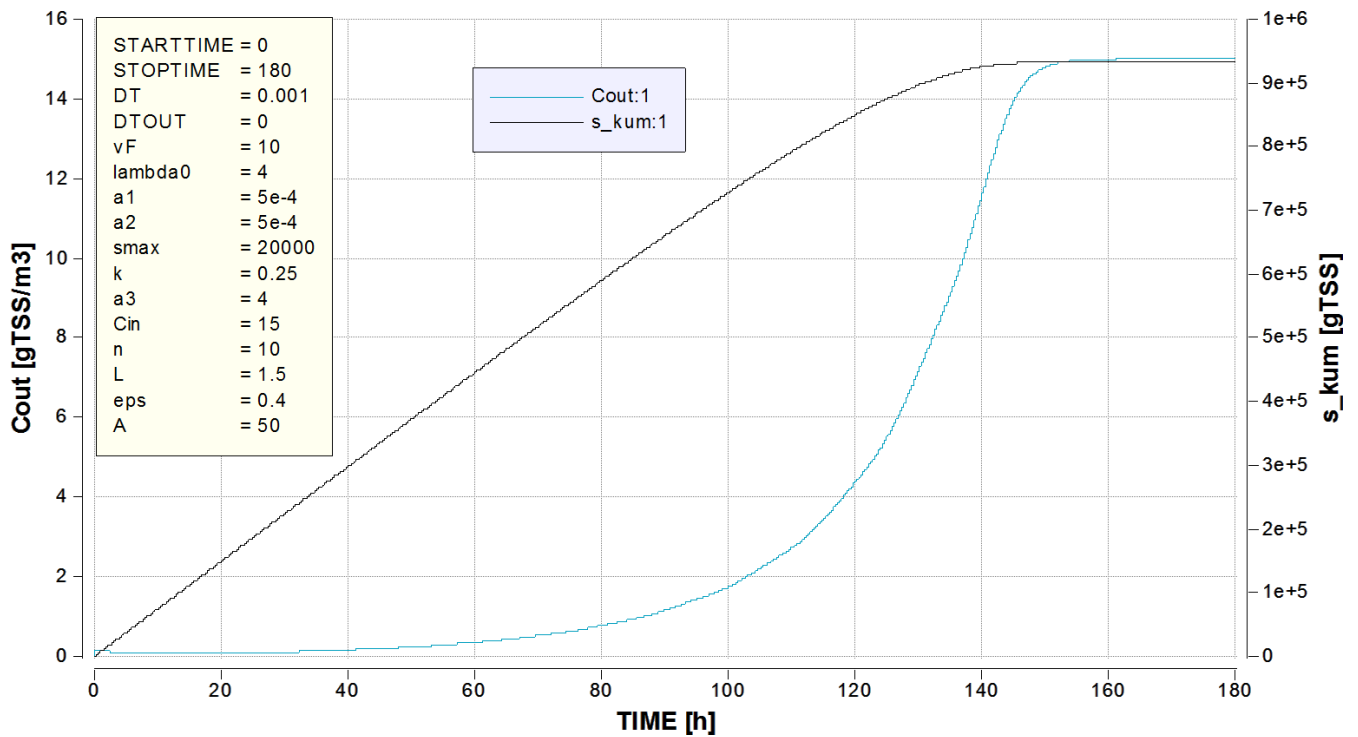


Figure 2: Development of the TSS effluent concentration and the total mass of accumulated solids over time.

The development of the total head loss over time is shown in Figure 3.

It can be concluded that the total head loss is the limiting criteria to determine backwashing of the filter since $t_{HL} < t_{Breakthrough}$.

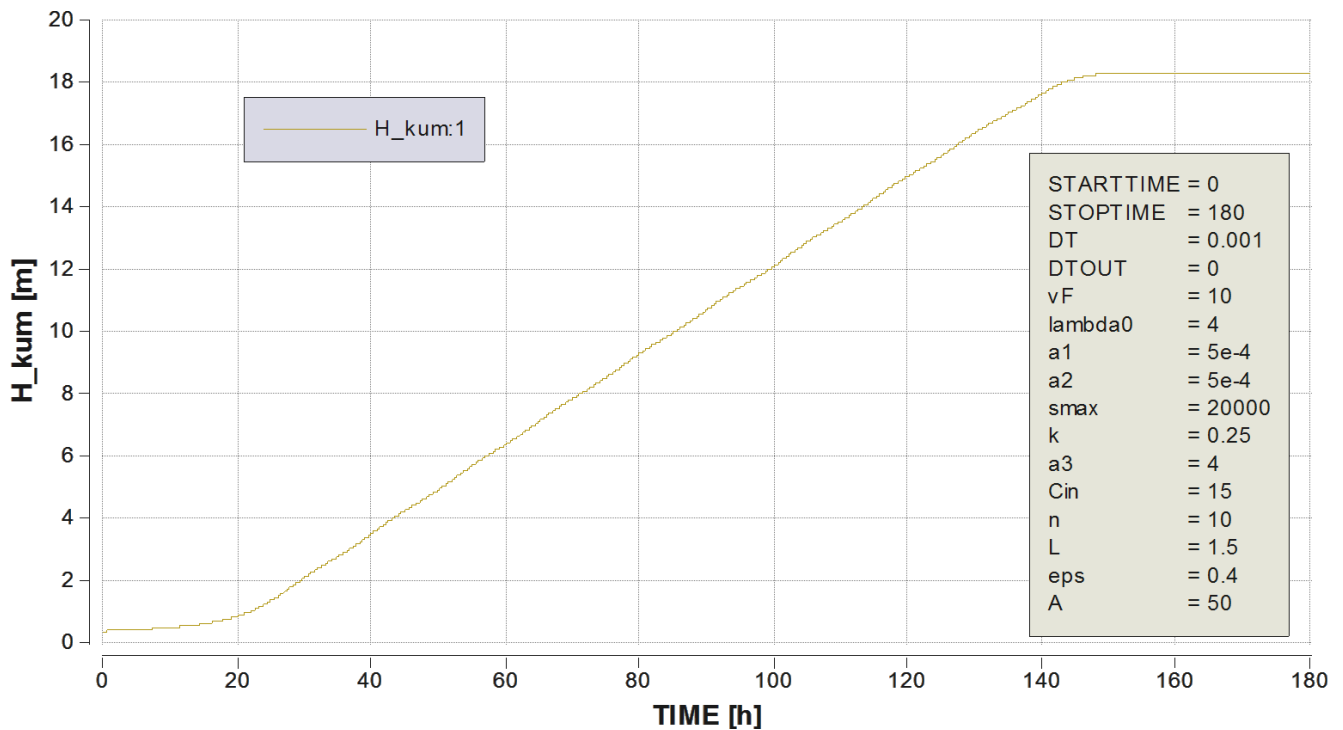
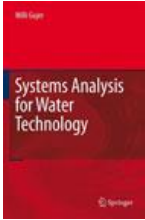


Figure 3: Development of total head loss H over time.



Substrate Profiles in a Biofilm

1. Concentration profile of ammonium over the depth of a nitrifying biofilm.

For numeric simulation of a biofilm, it is recommendable to start the z-axis at the substratum, so the surface of the biofilm is at its thickness L_F .

In order to solve the second order differential equation, two boundary conditions are needed:

$$\text{B.C.1} \quad S_{NH}(z = L_F) = S_{NH,surface} \quad (\text{measured})$$

$$\text{B.C.2} \quad S'(z = 0) = 0 \quad (\text{no substrate can diffuse into the substratum})$$

As can be seen in Figure 1, the ammonium concentration at the substratum ($z = 0$) is 0.687 gN/m^3 . This value is determined in BM with the help of Model > Modules > Boundary Value ODE: The boundary condition which is needed here is $S_{NH}(z=0.0005) = 3$ and corresponds to B.C.1, the parameter to adapt is $S_{NH,0}$ ($= S_{NH}(z=0)$).

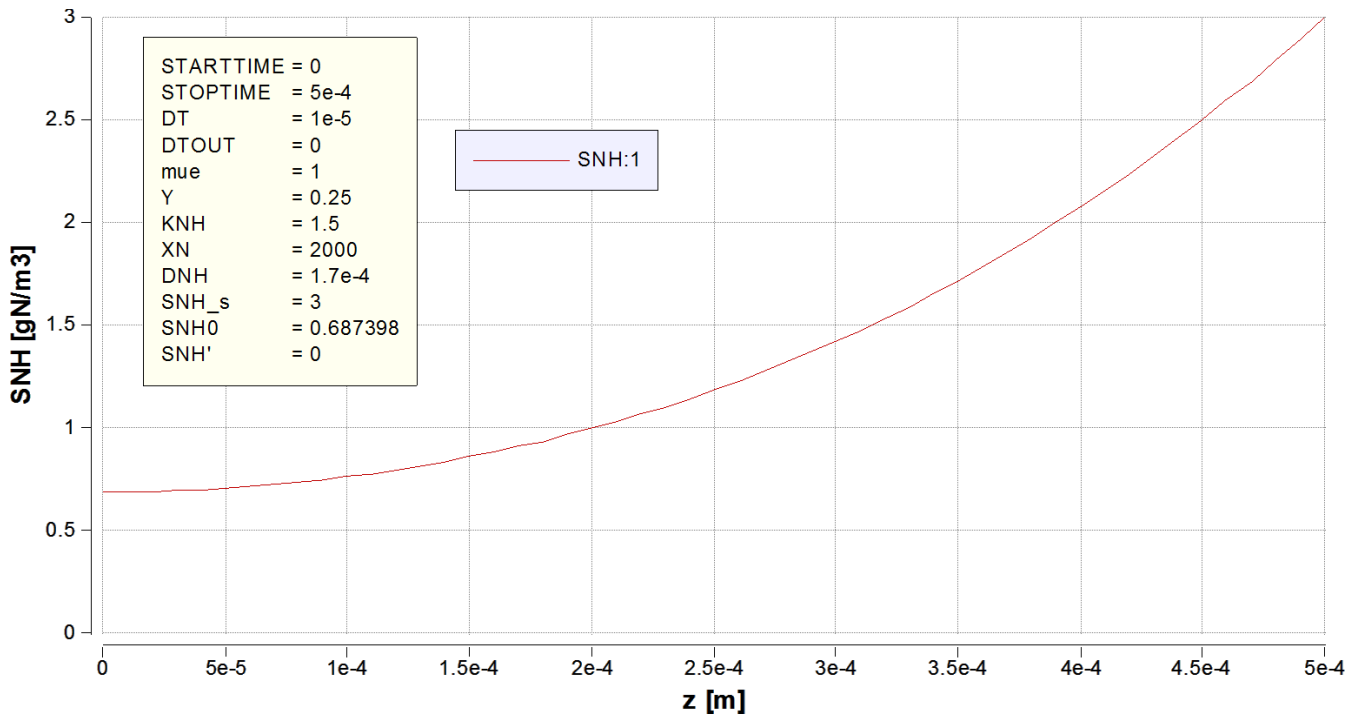


Figure 1: Concentration profile of ammonium over the depth of the biofilm ($L_F = 0.0005$ m).

The amount of ammonium that this biofilm can nitrify, can be approximated by determining the mass flux of ammonium:

$$j_{NH} = -D_{NH} * \frac{dS_{NH}}{dz}$$

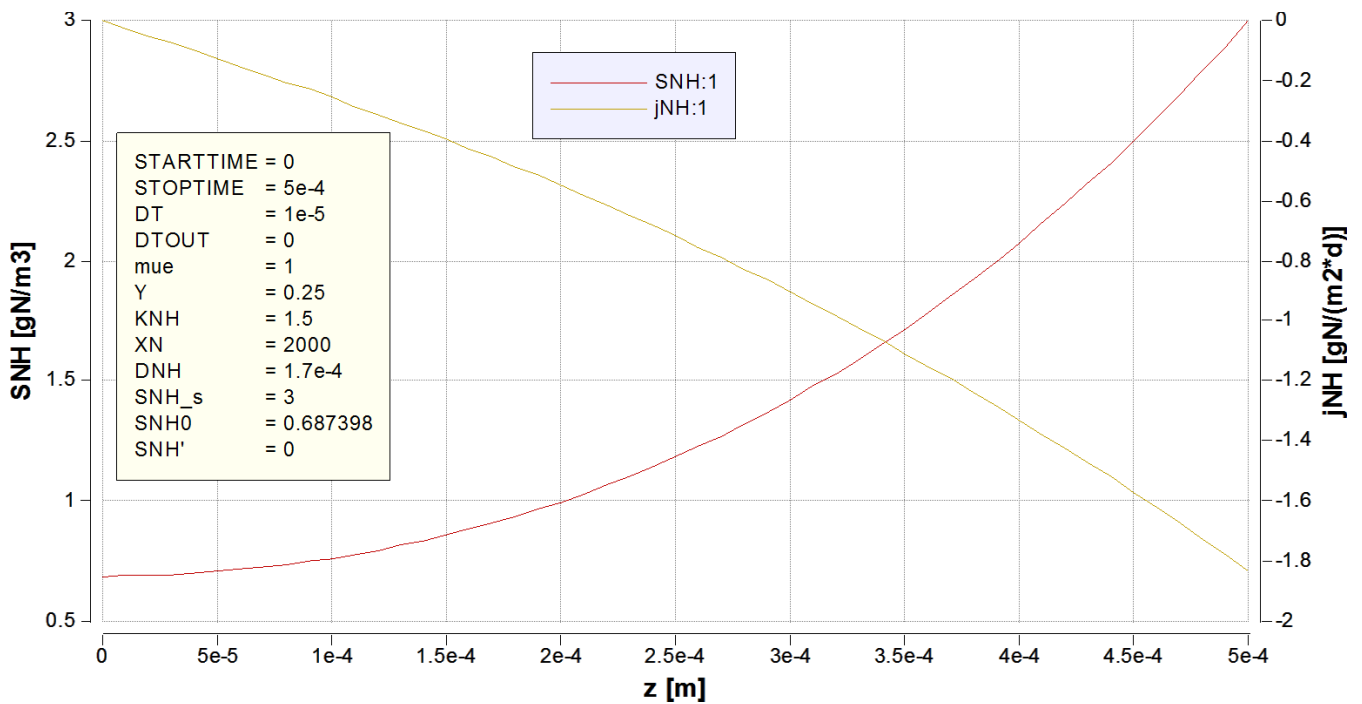


Figure 2: Ammonium mass flux in the biofilm and concentration profile over the biofilm thickness ($L_F = 0.0005$ m).

The flux of ammonium at the biofilm surface, $j_{NH}(z=L_F)$, is what is "consumed" from the bulk water:

$$j_{NH} = -D_{NH} * \frac{dS_{NH}}{dz} \rightarrow j_{NH}(z = L_F) = j_{NH,surface} = -1.83 \frac{gN}{m^2 * d}$$

Alternatively, one can look at the ammonium consumption rate r_{NH} , integrated over the thickness of the biofilm L_F , as shown in Figure 3:

$$\frac{dj_{NH}}{dz} = r_{NH} \rightarrow j_{NH,surface} = -1.83 \frac{gN}{m^2 * d}$$

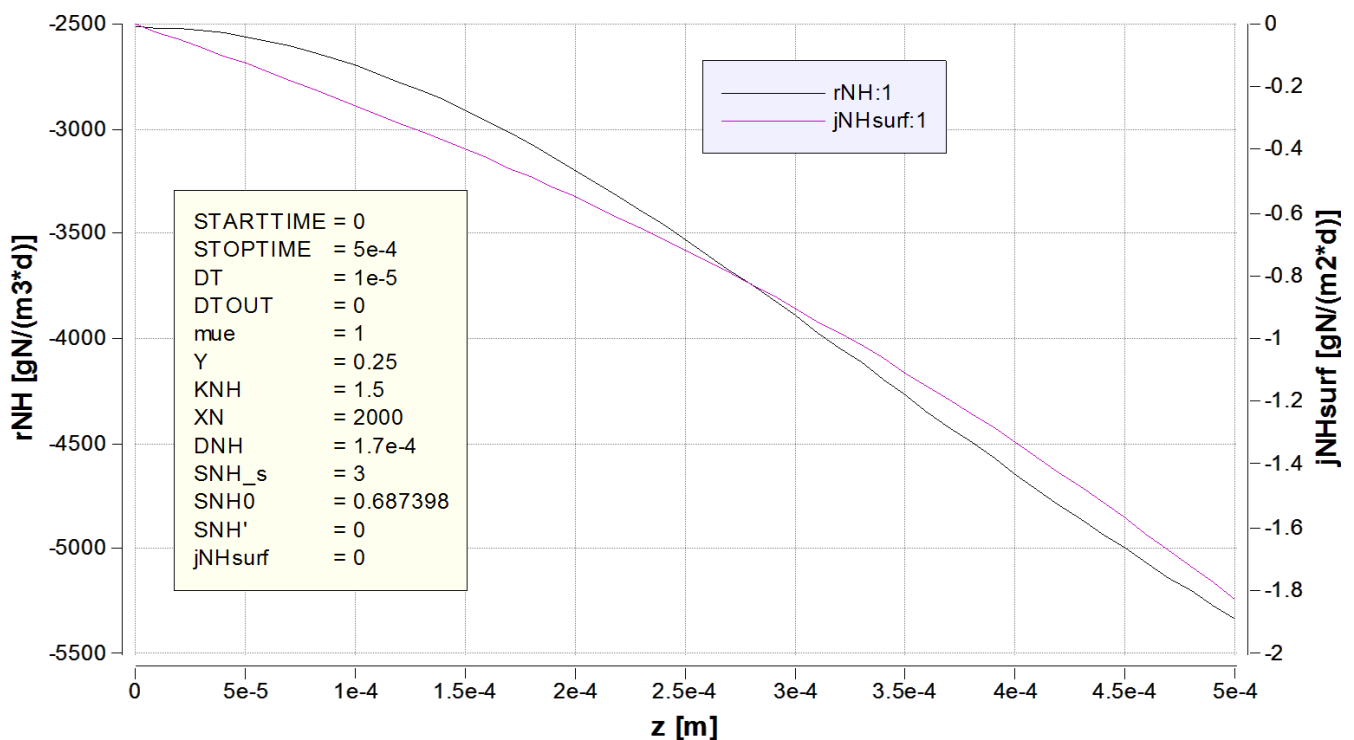


Figure 3: Ammonium consumption rate and ammonium mass flux in the biofilm.

2. Ammonium, nitrate and oxygen concentration profiles.

From Figure 4, the following concentrations at the substratum ($z = 0$) for ammonium, nitrate and oxygen, respectively, can be read:

$$S_{NH,0} = 1.01 \text{ gN/m}^3$$

$$S_{O_2,0} = 0.76 \text{ gO}_2/\text{m}^3$$

$$S_{NO,0} = 4.11 \text{ gN/m}^3$$

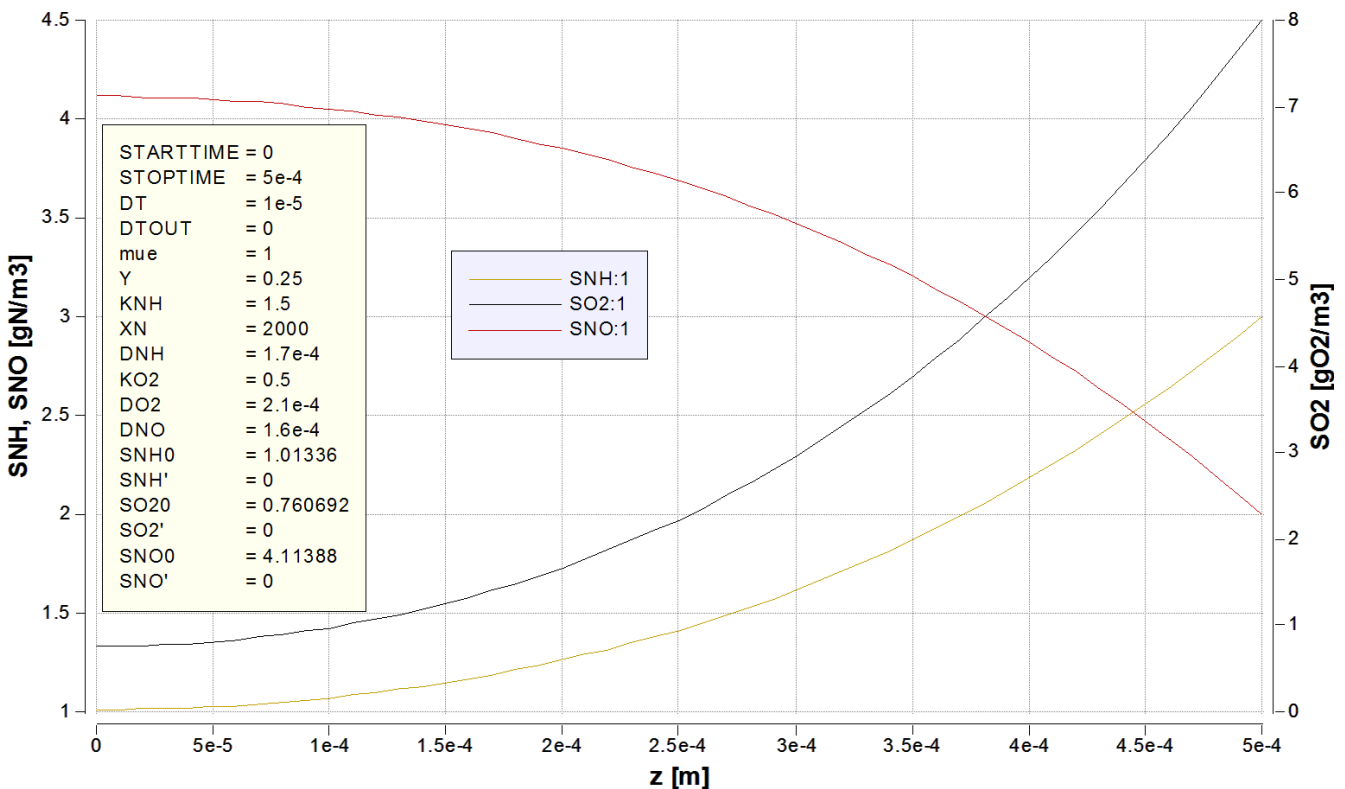


Figure 4: Concentration profiles of ammonium S_{NH} , nitrate S_{NO} and oxygen S_o over the biofilm thickness ($L_F = 0.0005 \text{ m}$).

The nitrification rate can be limited either by the electron donor (ammonium) or by the electron acceptor (oxygen). Which case applies for a given system can be evaluated with the help of the following equation¹:

¹ Equation 17.87 from: Eberhard Morgenroth. Biological Wastewater Treatment: Principles, Modelling and Design. 2008. IWA Publishing, London, UK.

$$\gamma_{NH, O_2} = \sqrt{(\alpha - Y) * \frac{D_{NH} * S_{NH, surface}}{D_{O_2} * S_{O_2, surface}}} \quad \text{with } \alpha = 4.57 \frac{gO_2}{gN} \text{ for nitrification}$$

Case 1: $\gamma_{NH, O_2} < 1$ -> ammonium is potentially limiting

Case 2: $\gamma_{NH, O_2} > 1$ -> oxygen is potentially limiting

For the given biofilm system, it is the following ratio:

$$\gamma_{NH, O_2} = \sqrt{\left(4.57 \frac{gO_2}{gN} - 0.25 \frac{gCOD}{gN}\right) * \frac{1.7 * 10^{-4} \frac{m^2}{d} * 3 \frac{gN}{m^3}}{2.1 * 10^{-4} \frac{m^2}{d} * 8 \frac{gO_2}{m^3}}} = 1.15 > 1 \rightarrow O_2 \text{ is limiting.}$$

In other words, this means that we would need 1.15 times more oxygen diffusing into the biofilm to tap the full potential of ammonium nitrification.

This could also be seen from the oxygen and ammonium concentration at the substratum: ($S_{O_2,0} = 0.76 \text{ gO}_2/\text{m}^3$) \ll $(18/4 = 4.5 \text{ gO}_2/\text{gN}) * (S_{NH,0} = 1.01 \text{ gN}/\text{m}^3)$.

Another way to determine the limiting compound is with the help of the stoichiometric matrix. In subtask 1, we assumed that there would always be as much oxygen present in the biofilm as needed by nitrification. The potential amount of oxygen consumed is:

$$\Delta S_{O_2, pot} = \Delta S_{NH, pot} * \frac{v_{O_2}}{v_{NH}} = -(3 - 0.69) \frac{gN}{m^3} * \frac{-18 \frac{gO_2}{gN}}{-4 \frac{gN}{gN}} = 10.41 \frac{gO_2}{m^3}$$

In subtask 2, however, diffusion of oxygen is considered as well. The remaining ammonium concentration at the substratum is higher, which means that less oxygen was consumed. So the actual amount of oxygen consumed is:

$$\Delta S_{O_2, act} = \Delta S_{NH, act} * \frac{v_{O_2}}{v_{NH}} = -(3 - 1.01) \frac{gN}{m^3} * \frac{-18 \frac{gO_2}{gN}}{-4 \frac{gN}{gN}} = 8.96 \frac{gO_2}{m^3}$$

The ratio of the two oxygen consumption values corresponds to the above found γ_{NH, O_2} :

$$\frac{\Delta S_{O_2, pot}}{\Delta S_{O_2, act}} = 1.16 = \gamma_{NH, O_2}$$

To determine the turnover from the bulk liquid to the biofilm, one can look at the mass fluxes at the surface of the biofilm, because that is what is "consumed" (or "produced", in the case of nitrate) from the bulk water. The mass fluxes at the surface are for ammonium, oxygen and nitrate, respectively (see Figure 5):

$$j_{NH}(z=L_F) = - 1.63 \text{ gN}/(\text{m}^2 \cdot \text{d})$$

$$j_{O_2}(z=L_F) = - 7.34 \text{ gO}_2/(\text{m}^2 \cdot \text{d})$$

$$j_{NO}(z=L_F) = + 1.63 \text{ gN}/(\text{m}^2 \cdot \text{d})$$

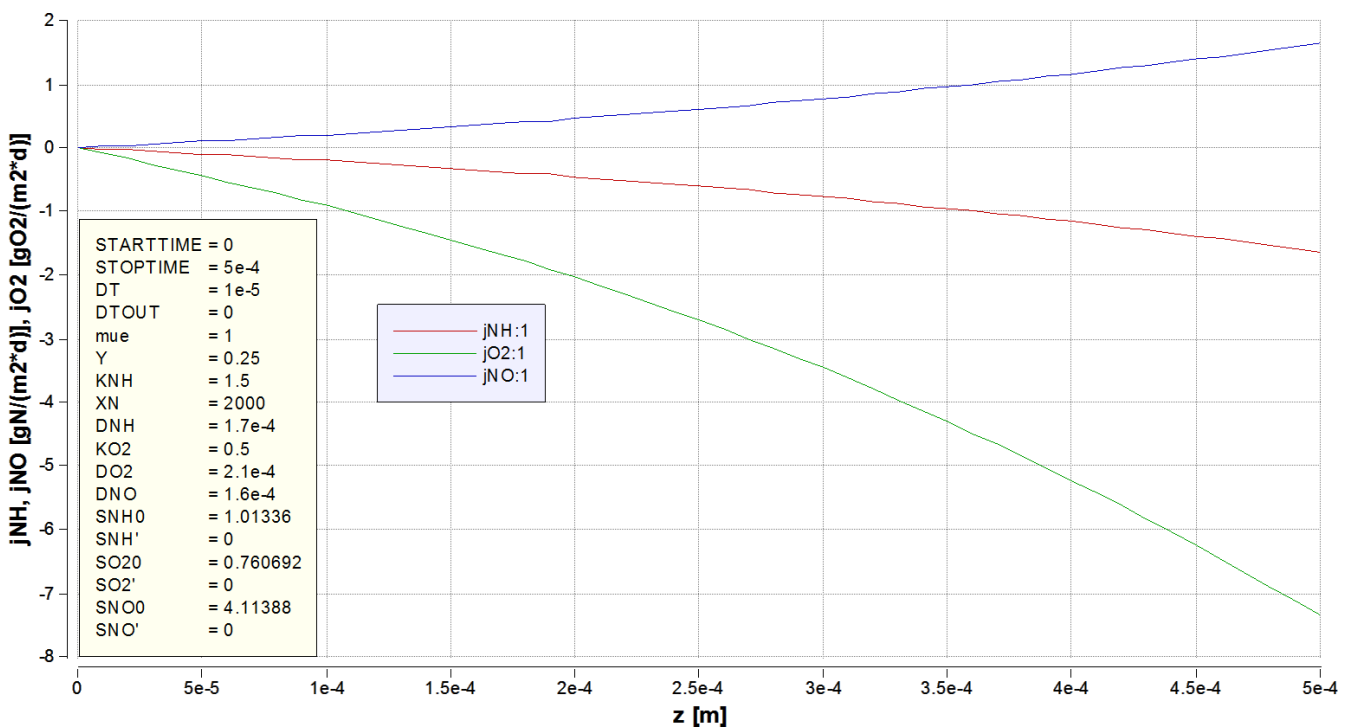


Figure 5: Mass fluxes of ammonium, nitrate and oxygen in the biofilm.

The fluxes of the three compounds are in relation to each other via the stoichiometric matrix:

$$j_{NH} = j_{O_2} * \frac{v_{NH}}{v_{O_2}} \quad e. g. j_{NH}(z = L_F) = -7.34 \frac{gO_2}{m^2 * d} * \frac{-4 \frac{gN}{gN}}{-18 \frac{gO_2}{gN}} = -1.63 \frac{gN}{m^2 * d}$$

$$j_{NO} = j_{O_2} * \frac{v_{NO}}{v_{O_2}} \quad e. g. j_{NO}(z = L_F) = -7.34 \frac{gO_2}{m^2 * d} * \frac{+4 \frac{gN}{gN}}{-18 \frac{gO_2}{gN}} = +1.63 \frac{gN}{m^2 * d}$$

3. Consideration of a laminar boundary layer – effect of external mass transfer resistance.

If we assume that there is a (linear) laminar boundary layer of $5 \cdot 10^{-5}$ m thickness at the surface of the biofilm, the transport of the three compounds from the bulk water to the biofilm is hindered. As a consequence, the concentration profiles for the three compounds will change (see Figure 6) since per definition, there is no reaction ($r = 0$) in the laminar boundary layer.

The resulting concentrations at the substratum ($z = 0$) for ammonium, nitrate and oxygen, respectively, can be read from Figure 6:

$$S_{NH,0} = 0.93 \text{ gN/m}^3$$

$$S_{O_2,0} = 0.45 \text{ gO}_2/\text{m}^3$$

$$S_{NO,0} = 4.20 \text{ gN/m}^3$$

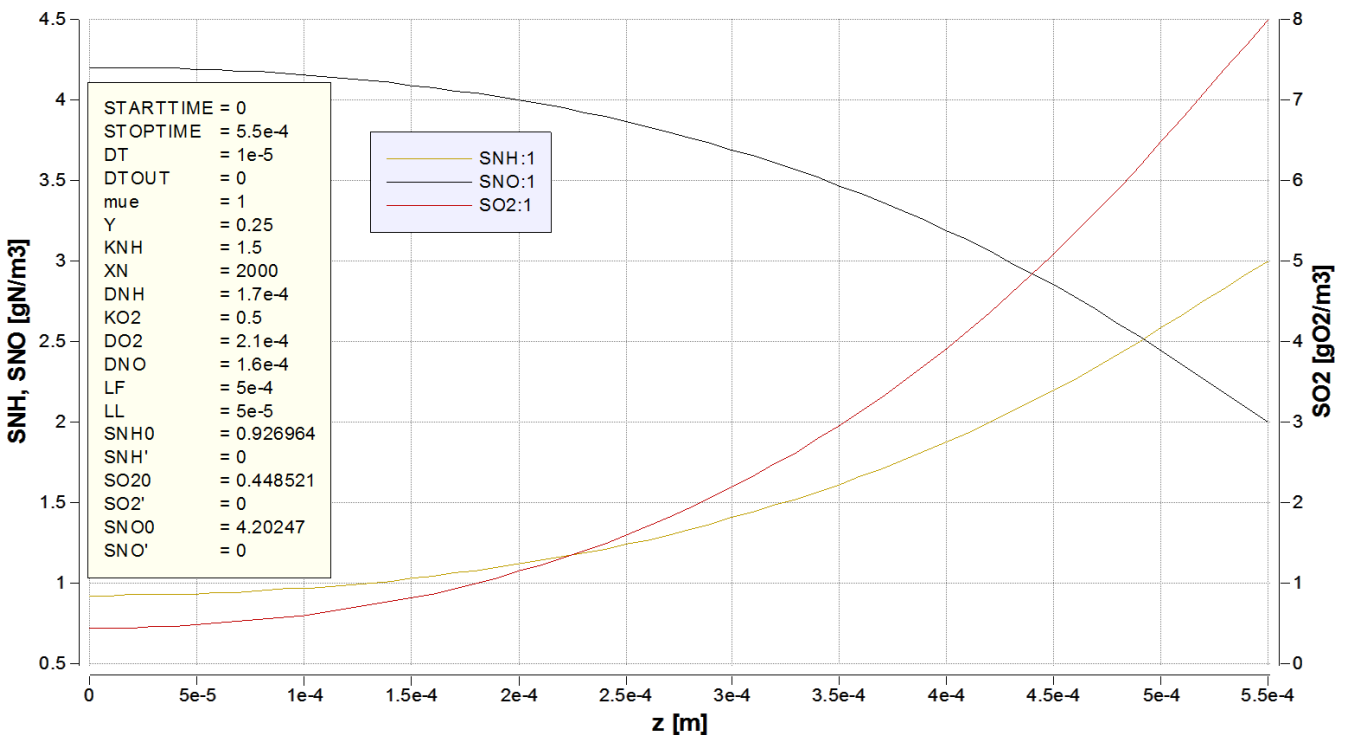


Figure 6: Concentration profiles of ammonium SNH, nitrate SNO and oxygen SO over the biofilm thickness plus laminar boundary layer thickness (= LF + LL = 0.00055 m).

The resulting fluxes of the three compounds through the biofilm and the laminar boundary layer are shown in Figure 7.

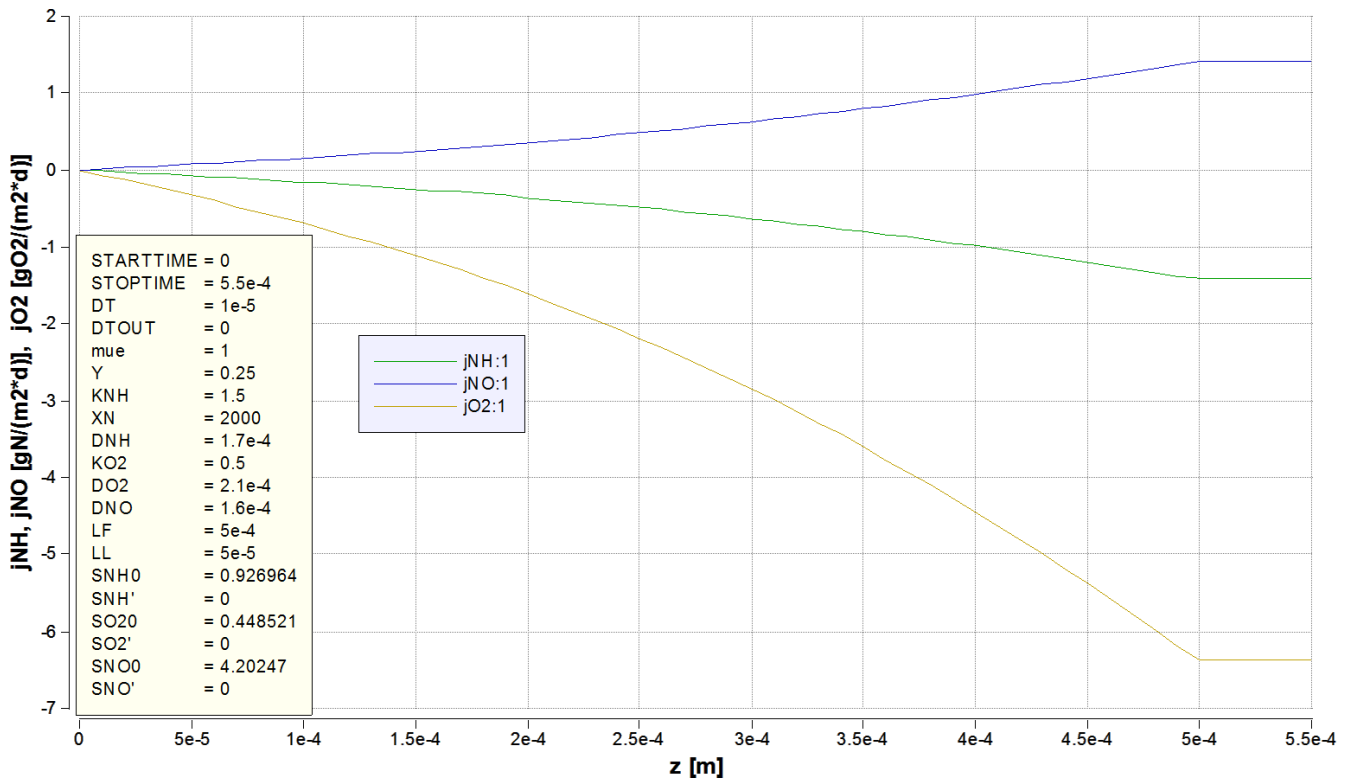


Figure 7: Mass fluxes of ammonium, nitrate and oxygen in the biofilm when considering a laminar boundary layer.

The flux across the laminar boundary layer, j_{BL} , is modeled by considering a mass transfer resistance, according to the following equation²:

$$j_{BL} = \frac{D_W}{L_L} * (S_B - S_{LF}) = k_C * (S_B - S_{LF})$$

D_W : Diffusion coefficient of compound in water [m^2/d], for simplification assumed here: $D_W \approx D_F$ (D_F : diffusion coefficient in biofilm [m^2/d], given)

L_L : Thickness of laminar boundary layer [m]

S_B : Bulk liquid concentration of compound [g/m^3]

S_{LF} : Concentration of compound at surface of biofilm (at $z=L_F$) [g/m^3]

k_C : External mass transfer coefficient [m/d]

² Equation 17.46 from: Eberhard Morgenroth. Biological Wastewater Treatment: Principles, Modelling and Design. 2008. IWA Publishing, London, UK.

The mass transfer coefficient across the boundary layer for each compound can be calculated in two ways:

$$k_{C,NH} = \frac{j_{BL,NH}}{(S_{B,NH} - S_{LF,NH})} = \frac{-1.41 \frac{gN}{m^2 * d}}{(3.00 - 2.58) \frac{gN}{m^3}} = \left| -3.36 \frac{m}{d} \right| \quad \text{or} \quad k_{C,NH} = \frac{D_{NH}}{L_L} = \frac{1.7 * 10^{-4} \frac{m^2}{d}}{0.00005 m} = 3.4 \frac{m}{d}$$

$$k_{C,O_2} = \frac{j_{BL,O_2}}{(S_{B,O_2} - S_{LF,O_2})} = \frac{-6.36 \frac{gO_2}{m^2 * d}}{(8.00 - 6.49) \frac{gO_2}{m^3}} = \left| -4.21 \frac{m}{d} \right| \quad \text{or} \quad k_{C,O_2} = \frac{D_{O_2}}{L_L} = \frac{2.1 * 10^{-4} \frac{m^2}{d}}{0.00005 m} = 4.2 \frac{m}{d}$$

$$k_{C,NO} = \frac{j_{BL,NO}}{(S_{B,NO} - S_{LF,NO})} = \frac{1.41 \frac{gN}{m^2 * d}}{(2.00 - 2.44) \frac{gN}{m^3}} = \left| -3.20 \frac{m}{d} \right| \quad \text{or} \quad k_{C,NO} = \frac{D_{NO}}{L_L} = \frac{1.6 * 10^{-4} \frac{m^2}{d}}{0.00005 m} = 3.2 \frac{m}{d}$$

Bode Diagram

1. Bode diagram for a plug-flow reactor and a cascade of 1, 2 or 6 CSTRs.

It is clearly visible in Figure 1 that the relative amplitudes for the effluent concentrations decrease in the following order: $A_{out}(1 \text{ CSTR}) > A_{out}(2 \text{ CSTRs}) > A_{out}(\text{PFR}) > A_{out}(6 \text{ CSTRs})$. In the case of CSTRs, the attenuation results from hydraulic attenuation (mixing) and degradation of the compound. Whereas in a PFR, the attenuation results from the degradation process only.

It can be concluded that for the given frequency ($f = 3 \text{ d}^{-1}$), the cascade of 6 CSTRs shows the best performance in terms of attenuation, however, in terms of compound removal, the PFR reaches the lowest absolute effluent concentration.

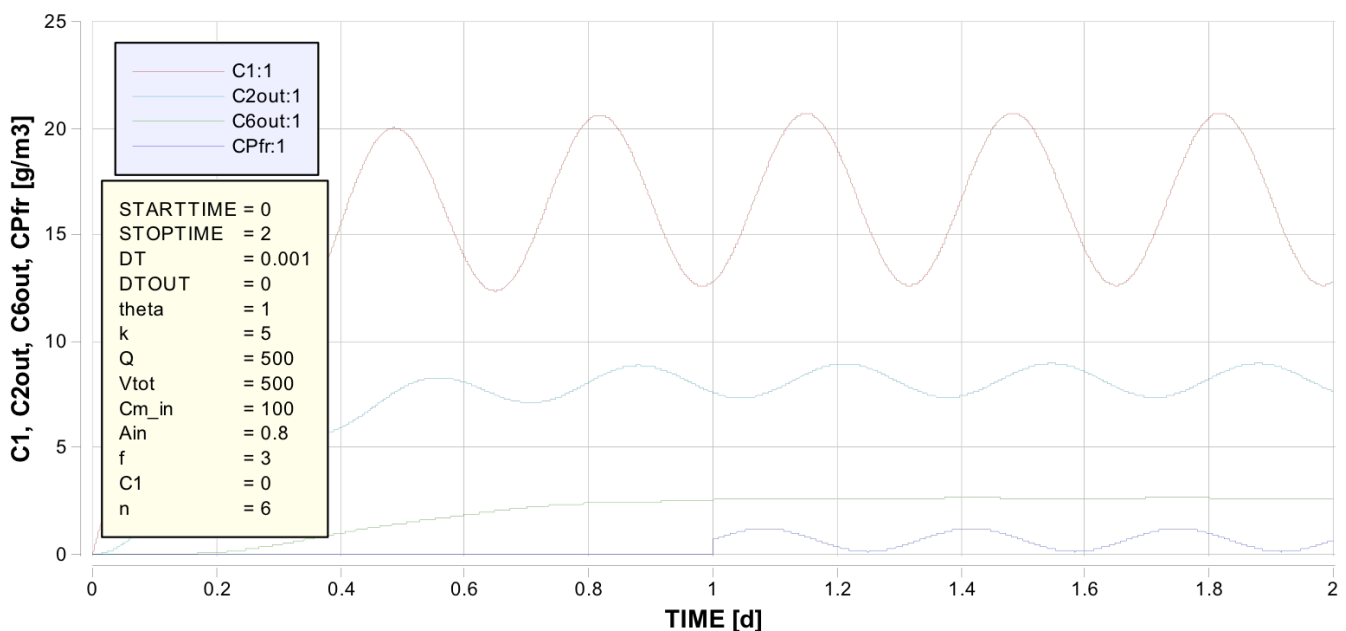


Figure 1: Effluent concentrations for a plug-flow reactor (CPfr), one CSTR (C1), a cascade of 2 CSTRs (C2) and a cascade of 6 CSTRs (C6) for sinusoidal concentration variations in the influent.

With the help of a Bode diagram, we can see the response of a reactor system to many different frequency values of the influent disturbance.

The Bode diagram in Figure 2 shows that the ideal PFR is in fact independent of the frequency f as there is no mixing effect in the reactor. For disturbances with small frequencies, the PFR shows the best performance. For higher frequencies, the performance of the cascade of 6 CSTRs is always superior compared to the other reactor configurations,

because it combines strong hydraulic damping and also degradation. Only for very high frequencies ($f \cdot \theta h \approx 30 \text{ d}^{-1}$), the single CSTRs reaches a better performance than the PFR.

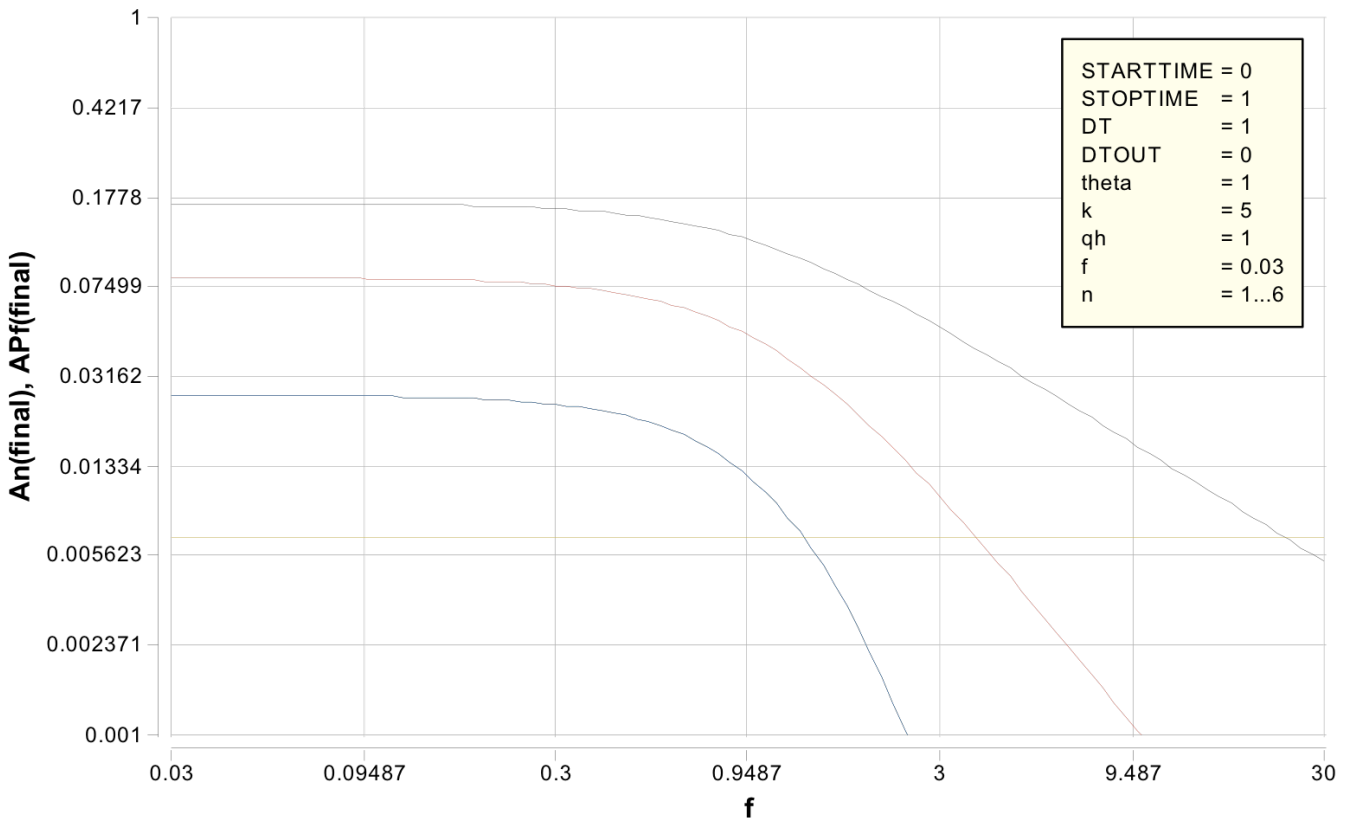


Figure 2: Bode diagram, created with Parameter plot (geometric) for $f = 0.03-30$ and $k \cdot \theta h = 5$. Legend: black: 1 CSTR, red: cascade of 2 CSTRs, blue: cascade of 6 CSTRs, yellow: ideal PFR. Note: Both axes are in log-scale.

Dynamic Nitrification

1. Required maximum growth rate of the nitrifiers

A flow scheme of the activated sludge plant under investigation is depicted in Figure 1. Sludge wasting (Q_{ex}) is done directly from the aeration tank in order to achieve a solids retention time (SRT) of 5.3 days. It is assumed that there are no solids in the effluent. For the first task, only the aeration tank is of importance, the secondary clarifier can be modeled as described in the hints in BM. The code is shown below.

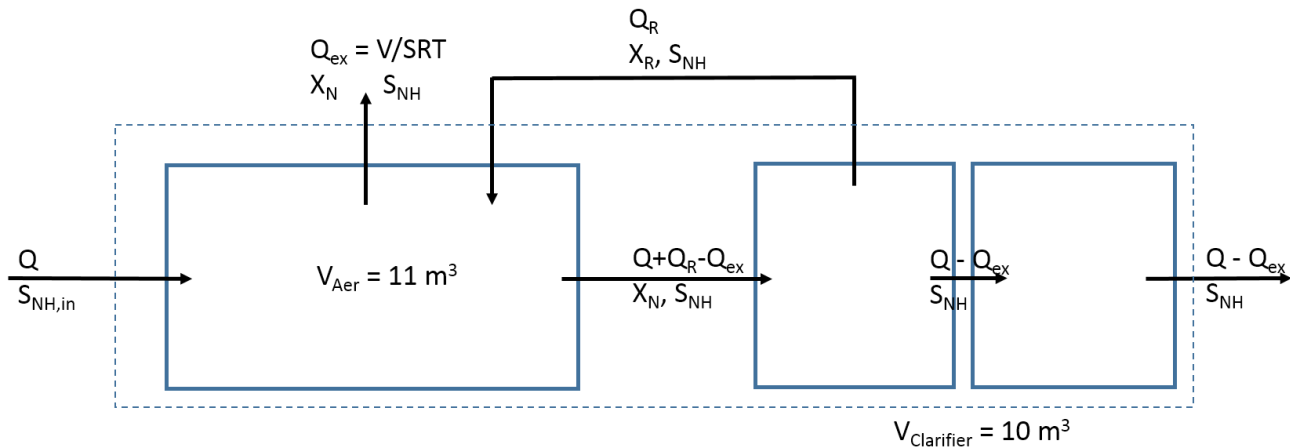


Figure 1: Flow scheme of the activated sludge plant with SRT = 5.3 d.

The corresponding mass balances for the aeration tank (CSTR) for the ammonium concentration S_{NH} and the nitrifier biomass X_N are as follows:

$$\begin{aligned} \frac{dS_{NH}}{dt} &= \frac{1}{V_{Aer}} * (Q * S_{NH,in} - (Q - Q_{ex} + Q_R) * S_{NH} - Q_{ex} * S_{NH} + Q_R * S_{NH}) - \frac{\mu_N}{Y_N} * \frac{S_{NH}}{K_{NH} + S_{NH}} * X_N \\ &= \frac{Q}{V_{Aer}} * (S_{NH,in} - S_{NH}) - \frac{1}{Y_N} * \mu_N * \frac{S_{NH}}{K_{NH} + S_{NH}} * X_N \end{aligned}$$

$$\frac{dX_N}{dt} = -\frac{Q_{ex}}{V_{aer}} * X_N + \mu_N * \frac{S_{NH}}{K_{NH} + S_{NH}} * X_N - b_N * X_N$$

Using the model you can find out that the required maximum growth rate μ_N of the nitrifiers is about 0.5 d^{-1} .

METHOD RK4

STARTTIME = 0
 STOPTIME = 100 ; Time in d
 DT = 0.001

;===Plant parameters, kinetics===

SRT = 5.3 ; Sludge retention time, d
 Temp = 14 ; Temperature, °C
 Vaer = 11 ; Volume aeration tank, m3
 mueN = 0.5 ; Maximum growth rate of the nitrifiers, d⁻¹ - TO ADAPT
 KNH = 1 ; Saturation coefficient for ammonium, gN/m3
 bN = 0.1*mueN ; Decay rate of the nitrifiers, d⁻¹
 YN = 0.24 ; Nitrifier yield coefficient, gCOD/gN
 Qex = Vaer/SRT ; Excess sludge, directly removed from the aeration tank, m3/d

SNHin = #SNH4(24*MOD(TIME,1)) ; Ammonium influent concentration, gN/m3
 Q = #FlowQd(24*MOD(TIME,1)) ; Inflow, m3/d

;===Mass balances===

init SNH = 1
 $d/dt(SNH) = Q/Vaer*(SNHin - SNH) - mueN*SNH/(KNH+SNH)*XN/YN$

init XN = 75
 $d/dt(XN) = -Qex/Vaer*XN + mueN*SNH/(KNH+SNH)*XN - bN*XN$

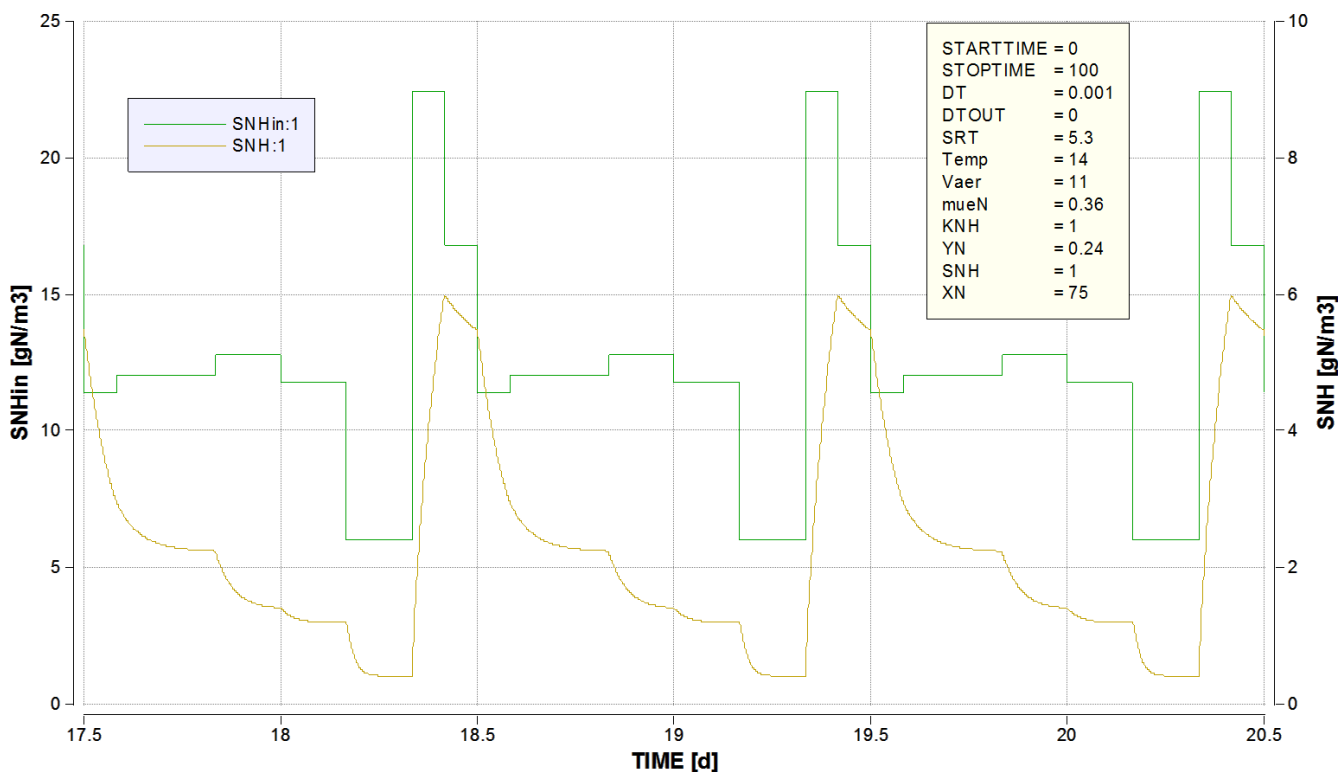


Figure 2: Ammonium concentration in the influent and the effluent of the aeration tank (CSTR).

2. Impact of secondary clarifier as a sequence of two CSTRs

If the secondary clarifier is modelled as a sequence of two CSTRs, the impact on the ammonium concentration is quite dramatic. As can be seen in Figure 3, the consequences of the secondary clarifier are an attenuation of the extremes (smaller amplitude) and also a delay of the peaks.

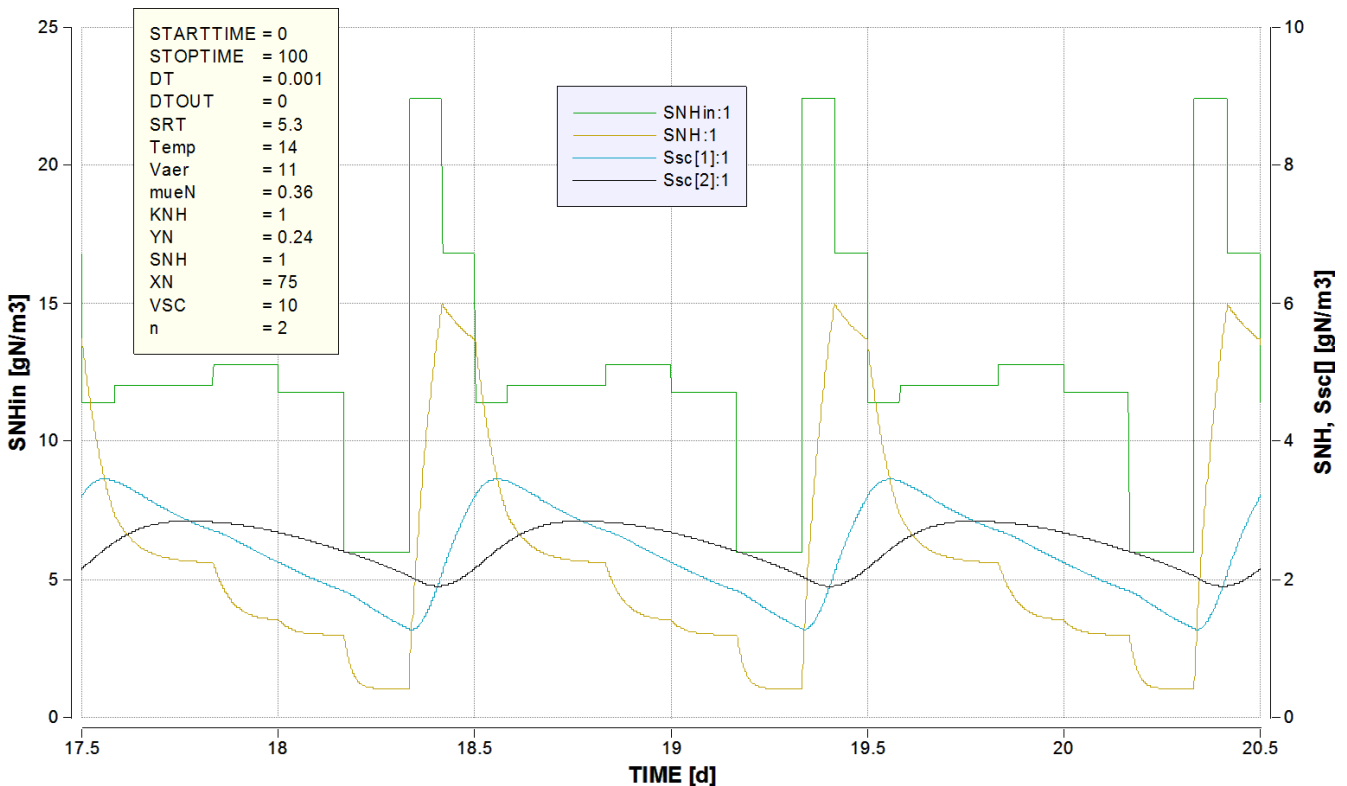


Figure 3: Ammonium concentration in the influent ($S_{NH,in}$) and the effluent (S_{NH}) of the aeration tank (CSTR) and in the effluent ($S_{Sc,1}$ and $S_{Sc,2}$) of the secondary clarifier (sequence of 2 CSTRs).

The code below needs to be added to the code of task 1 to model the secondary clarifier

```
VSC = 10           ; Volume secondary clarifier,m3
n = 2

init Ssc[1..2] = 1
d/dt(Ssc[1]) = (Q-Qex)*(SNH-Ssc[1])/Vsc/n
d/dt(Ssc[2..n]) = (Q-Qex)*(Ssc[i-1] - Ssc[i])/Vsc/n
```


3. Aeration tank as cascade of 3 CSTRs

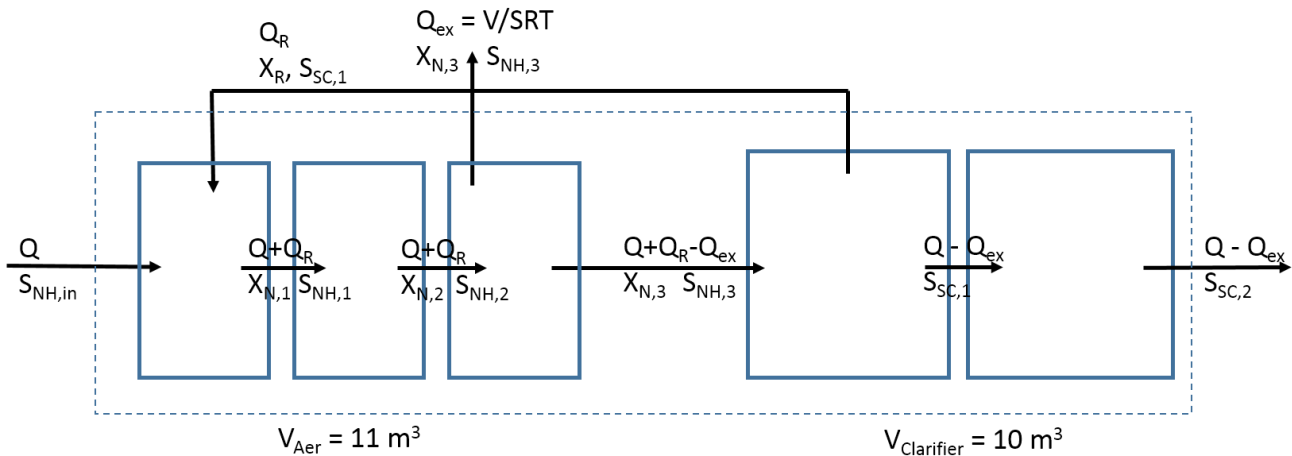


Figure 4: Adapted flow scheme of the activated sludge plant with SRT = 5.3 d.

If the aeration tank is modelled as a cascade of three equal CSTRs and the clarifier is kept as a sequence of two CSTRs (see Figure 4), there is some improvement on plant performance but not really substantial. The reason is that the ammonium concentrations are either rather high (higher than K_{NH}) or very low and therefore Monod kinetics is not very important.

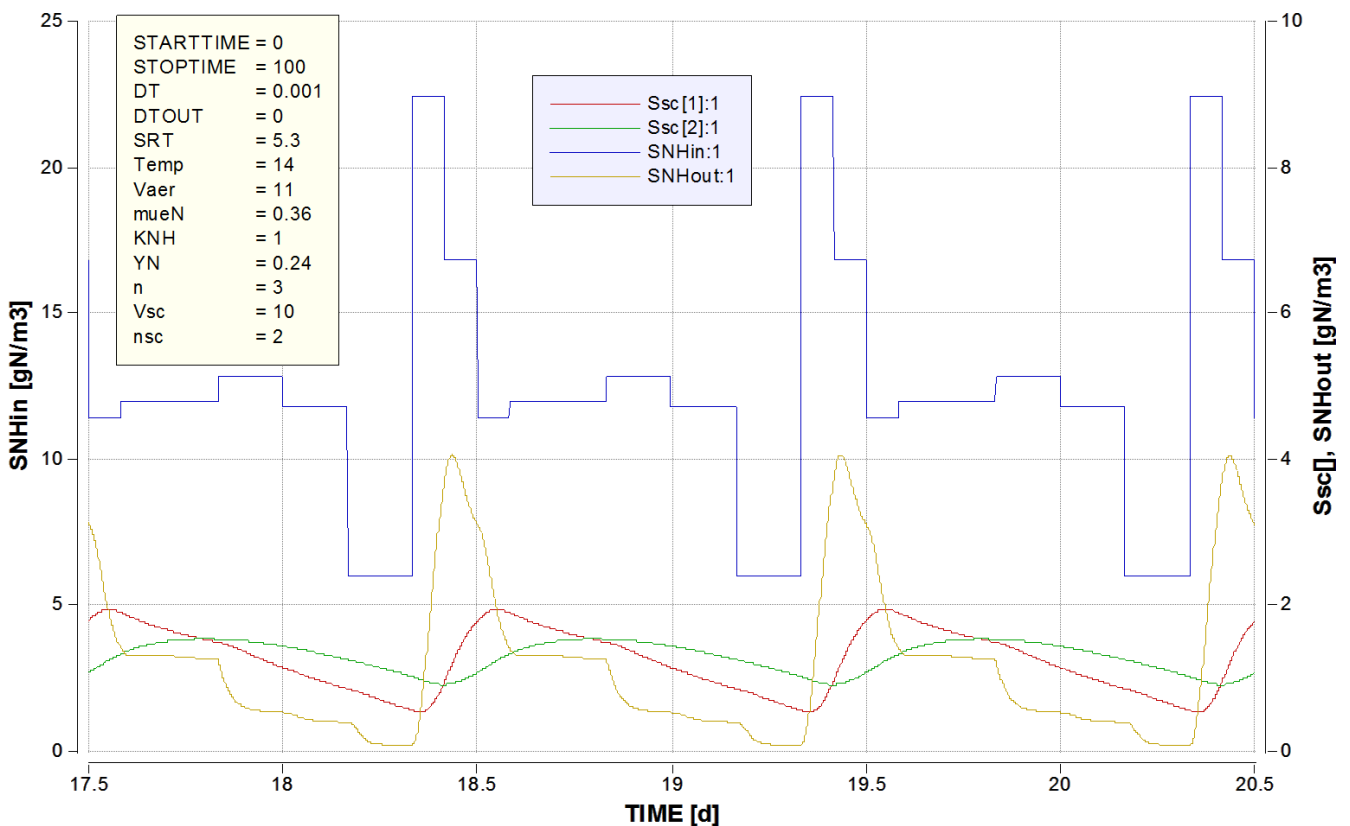


Figure 5: Ammonium concentration in the influent ($S_{NH,in}$) and the effluent ($S_{NH,out}$) of an aeration tank (sequence of 3 CSTRs) and in the effluent ($S_{sc,1}$ and $S_{sc,2}$) of the secondary clarifier (sequence of 2 CSTRs).

For the model the mass balances of the aeration reactor have to be adapted:

```
;===Mass balances===
```

```
n = 3
```

```
{ Sludge is removed from the last reactor }
```

```
V = Vaer/n
```

```
R = Q
```

```
init SNH[1..n] = 1
```

```
d/dt(SNH[1]) = (Q*SNHin + R*Ssc[1] - (Q+R)*SNH[i])/V - mueN*SNH[i]/(KNH+SNH[i])*XN[i]/YN
```

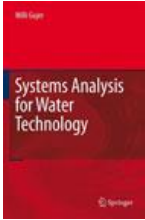
```
d/dt(SNH[2..n]) = (Q+R)*(SNH[i-1] - SNH[i])/V - mueN*SNH[i]/(KNH+SNH[i])*XN[i]/YN
```

```
init XN[1..n] = 85
```

```
d/dt(XN[1]) = (R*XNR - (Q+R)*XN[i])/V + mueN*SNH[i]/(KNH+SNH[i])*XN[i] - bN*XN[i]
```

```
d/dt(XN[2..n]) = (Q+R)*(XN[i-1]-XN[i])/V + mueN*SNH[i]/(KNH+SNH[i])*XN[i] - bN*XN[i]
```

```
XNR = (Q-Qex+R)*XN[n]/R
```



Nonstationary Flow in Sewers

1. Flow velocity at steady state

A sewer of 1000 m length is to be modelled as a series of nonlinear reservoirs, which are completely mixed reactors with a variable effluent Q_i . The length of one sewer section Δx is defined as 1 m here.

The resulting flow velocity at steady state is computed in the following way:

$$v_{stSt} = \frac{L}{V_{tot}/Q} = \frac{1000 \text{ m}}{130 \text{ m}^3 / 0.1 \text{ m}^3/\text{s}} = 0.77 \frac{\text{m}}{\text{s}}$$

2. Amplitude of the pollutant load during rain event

The amplitude of the pollutant load in the influent is zero (see Figure 1) since the changes of the flow rate Q and concentration C are in the opposite direction and compensate each other: due to the rainfall, Q increases whereas C is diluted by the additional water volume and therefore decreases.

The output pollutant load, however, shows an amplitude of +0.1 and -0.05 g/s, which is quite large. As can be seen in Figure 2, the water wave moves faster than the mass of pollutants, which causes the deformation of the pollutant load in the sewer.

The first increase in the pollutant load is caused by the rise of the flow rate, the drop in concentration happens a bit later and reduces the pollutant load again. The second amplitude in the pollutant load is due to a drop in the flow rate which again happens first, then the pollutant concentration rises which results in the initial level of the pollutant load.

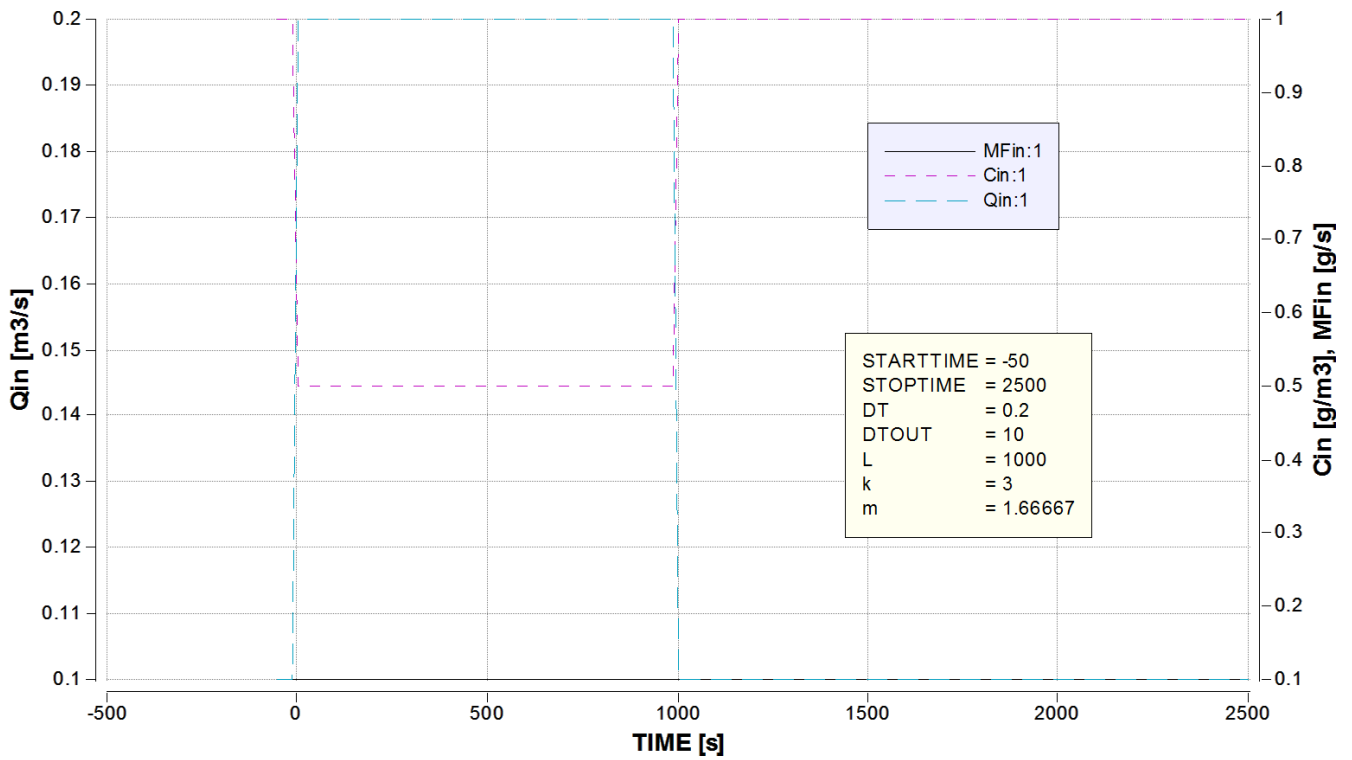


Figure 1: Flow rate Q , concentration C and pollutant load MF (mass flux) in influent during the rain event.

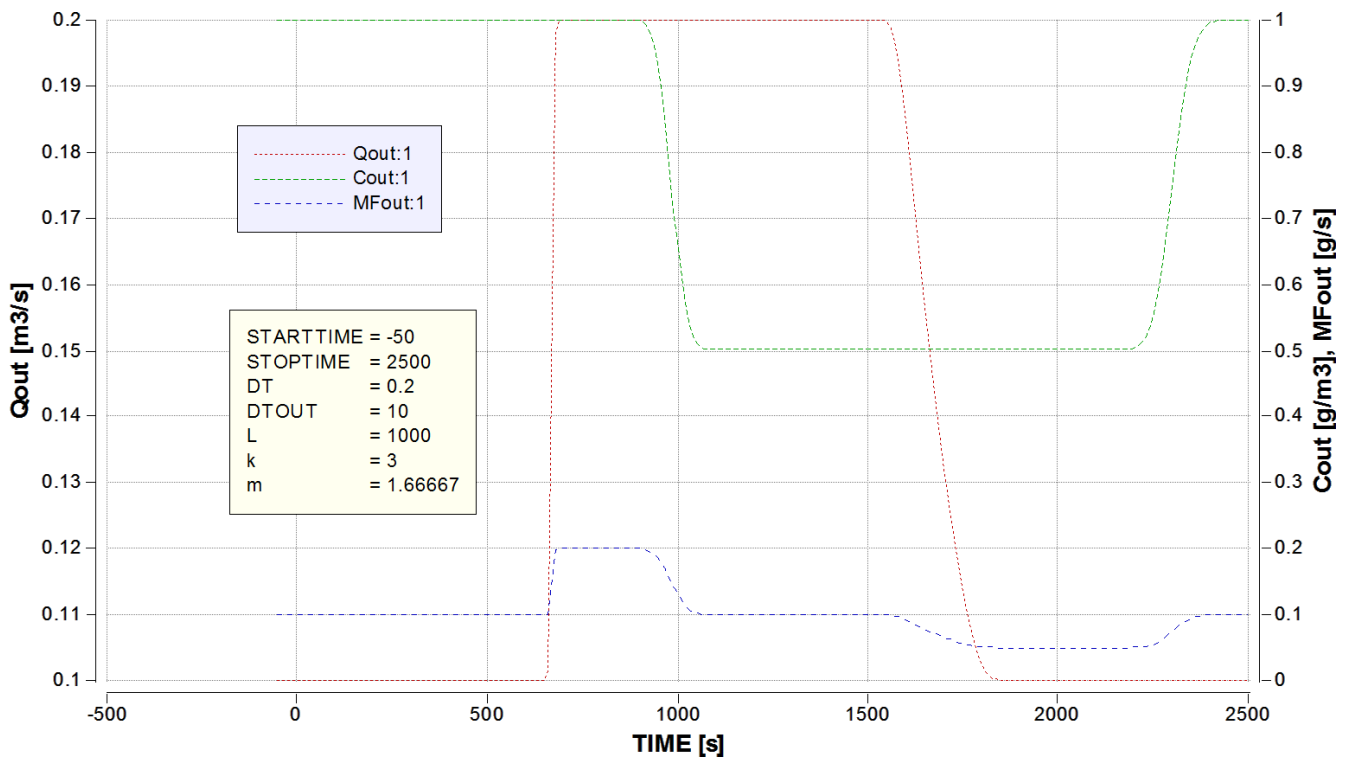


Figure 2: Flow rate Q , concentration C and pollutant load MF (mass flux) in the last reservoir (after a flow distance of $x = 1000$ m).

3. Maximum flow velocity and wave velocity during rain event

During the rain event, the flow rate is $Q_{\text{Rain}} = 0.2 \text{ m}^3/\text{s}$.

Flow velocity (velocity of pollutant mass):

$$v_{\text{max}} = \frac{L}{V_{\text{tot,max}}/Q_{\text{Rain}}} = \frac{1000 \text{ m}}{197 \text{ m}^3 / 0.2 \text{ m}^3/\text{s}} = 1.0 \frac{\text{m}}{\text{s}}$$

Wave velocity (celerity):

$$c_{\text{max}} \approx \frac{5}{3} * v_{\text{max}} = 1.7 \frac{\text{m}}{\text{s}}$$

The numeric model with the linear reservoirs yields slightly different values. As read from Fig. 2 we obtain:

The wave velocity (celerity) becomes: $c = 1000 \text{ m} / 666 \text{ sec} = 1.5 \text{ m s}^{-1}$

The flow velocity becomes: $v = 1000 \text{ m} / 985 \text{ sec} = 1 \text{ m s}^{-1}$

666s is the time when Q_{out} rises and 985s is the time when the concentration C_{out} decreases (see Fig.2).

Systematic Measurement Error

1. Plausibility check

To check the plausibility of the data two mass balances can be done. The first one is that of water and it can directly be seen that the values fit together.

$$Q_{in} - Q_{out} - Q_{Sludge} = 0$$

The plant probably only has a measurement of the influent and of the sludge removal, but not of the effluent. So the effluent value was just calculated from the two measurements.

The other mass balance is that of Phosphorous. Phosphorous only enters the system via the influent and only leaves it via the outflow or the sludge. It is not converted into any gaseous species that could leave the system in another way, unlike Nitrogen, so all the flows of Phosphorous can be measured.

$$\begin{aligned} m_{P,in} - m_{P,out} - m_{P,sludge} & \stackrel{!}{=} 0 \\ Q_{in} \cdot C_{P,in} - Q_{out} \cdot C_{P,out} - Q_{Sludge} \cdot C_{P,sludge} \\ & = 30 \frac{kg}{d} - 4.8 \frac{kg}{d} - 35 \frac{kg}{d} = -9.8 \frac{kg}{d} \end{aligned}$$

This result shows that either the flow or the phosphorus concentration or both measurements are not plausible.

2. Estimate of average flow rate

The measurement of the sludge volume is presumably more controlled than the influent as the following sludge treatment depends on it. This is also the case when the sludge is transported to another facility as then the WWTP has to pay for it. So we assume that this measurement is correct and the inflow is not, as is also stated in the description of the exercise.

Compared to flow measurements the concentration measurements are a lot more reliable and they can be assumed to be correct (they are regularly checked by state laboratories). We can use a mass balance to calculate the inflow rate.

$$Q_{in} \cdot C_{P,in} - Q_{out} \cdot C_{P,out} - Q_{Sludge} \cdot C_{P,Sludge} = 0$$

$$Q_{out} = Q_{in} - Q_{Sludge}$$

$$Q_{in} = \frac{Q_{Sludge}(C_{P,Sludge} - C_{P,out})}{C_{P,in} - C_{P,out}} = 8327 \frac{m^3}{d}$$

The value estimated by this simple calculation is nearly 40% higher than the one measured. With this estimation the inflow is a lot closer to the real inflow rate, which the recalibration found out to be 33% higher than assumed, and is therefore quite an improvement.

3. Conclusion

This exercise shows that an engineer shouldn't trust measurements, especially flow measurements, and that some errors can be found with a small effort and some simple calculations. A simple mass balance could have prevented the wrong dimensioning of the filter in the example described in the exercise.

Error Propagation with Correlated Uncertainty

Remark: Both influents in Figure 16.8 are called Influent A. In the following the lower one will be called Influent B.

1. Load of the wastewater treatment plant

To calculate the load of the wastewater treatment plant the following equation is used

$$L_{ww} = Q_A \cdot COD_A + Q_B \cdot COD_B = 13500 \frac{kg}{d}$$

For the computation of the uncertainty of the load we take the partial derivatives with respect to the concentrations of the two influents. As we assume that the influent flow rates are measured correctly we don't need to take into account their uncertainties.

$$\frac{\partial L_{ww}}{\partial COD_A} = Q_A \quad \text{and} \quad \frac{\partial L_{ww}}{\partial COD_B} = Q_B$$

The measurements of the COD concentrations are correlated. Therefore we need to use equation 12.27 and cannot simplify with Gaussian error propagation.

$$\sigma_L^2 = \left(\frac{\partial L_{ww}}{\partial COD_A} \right)^2 \cdot \sigma_{COD_A}^2 + \left(\frac{\partial L_{ww}}{\partial COD_B} \right)^2 \cdot \sigma_{COD_B}^2 + 2 \cdot \frac{\partial L_{ww}}{\partial COD_A} \cdot \frac{\partial L_{ww}}{\partial COD_B} \cdot r_{A,B} \cdot \sigma_{COD_A} \cdot \sigma_{COD_B} = 6.93 \cdot 10^{12} \frac{g^2}{d^2}$$

$$\sigma_L = 2632 \frac{kg}{d}$$

where σ are the standard deviations of the load and the concentrations, and $r_{A,B}$ is the correlation between the measurements of the concentrations in influents A and B.

Assuming a 95% confidence interval, which is given by approximately twice the standard deviation the expected value and its uncertainty are $L_{ww} = 13500 \pm 5265 kg/d$.

Due to the high correlation of the COD measurement error, the resulting error in the estimated combined COD load is nearly additive (and thus much larger than expected for the case without correlation).

2. Expected Error in Cost Contribution

As the errors of the COD measurements are positively correlated, the error of the cost contributions is smaller. This problem can be solved by a stochastic simulation. The correlation between the COD concentration in influent A and influent B can be implemented according to equations 12.40 and 12.41. Here the concentration in influent B is calculated depending on the concentration in influent A. The following code can be used in BM. It calculates the cost contribution for 10000 concentration combinations.


```
METHOD RK4
```

```
STARTTIME = 0  
STOPTIME=10001  
DT = 1
```

```
Qa = 10000  
CODa = normal(600,120)
```

```
{ see page 302, two correlated parameters }  
Qb = 15000  
CODb = 500 + (0.9*100/120)*(CODa-600)+normal(0,sigres)
```

```
sigres = ((1-0.9^2)*100^2)^0.5
```

```
CostA = 1E6*(Qa*CODa)/(Qa*CODa+Qb*CODb)  
CostB = 1E6*(Qb*CODb)/(Qa*CODa+Qb*CODb)
```

The results can be exported in Excel and mean and standard deviation can be calculated. As an alternative some additional lines of code can calculate these values directly in BM, as is shown below.

```
DTout = 10001 ; this simplifies reading the results in the output  
  
init CA[1..10000] = 0  
next CA[1..10000] = if time = i then CostA else CA[i] ; this stores the results in an array  
init CB[1..10000] = 0  
next CB[1..10000] = if time = i then CostB else CB[i]  
  
meanCostA = if time < stoptime then 0 else arraymean(CA[*]) ; compute mean and standard deviation once  
stdevCostA = if time < stoptime then 0 else arraystddev(CA[*])  
  
meanCostB = if time < stoptime then 0 else arraymean(CB[*])  
stdevCostB = if time < stoptime then 0 else arraystddev(CB[*])
```

The error of the cost contributions is relatively small compared to the total costs, around 24'000€ per year (2.4%), and the mean values are around 445'000€ per year for influent A and 555'000€ per year for influent B.

Uncertainty, Error Propagation

1. Resulting uncertainty (neglecting uncertainty from hydraulic model)

The ozone disinfection reactor from problem 16.9 is now modelled in consideration of the uncertainties of the different model parameters. In a first step, the uncertainty stemming from the hydraulic model (n , V) is neglected, so only the uncertainties of the following parameters are considered: Flow rate Q , ozone concentration $S_{O_3,1}$ and the reaction rates k_{O_3} and k_D .

Gaussian error propagation:

The steady state effluent concentration of the bacteria X_B is $1.33 \cdot 10^{-6}$ #/m³ (see Figure 1), this corresponds to a fraction of 0.000133%.

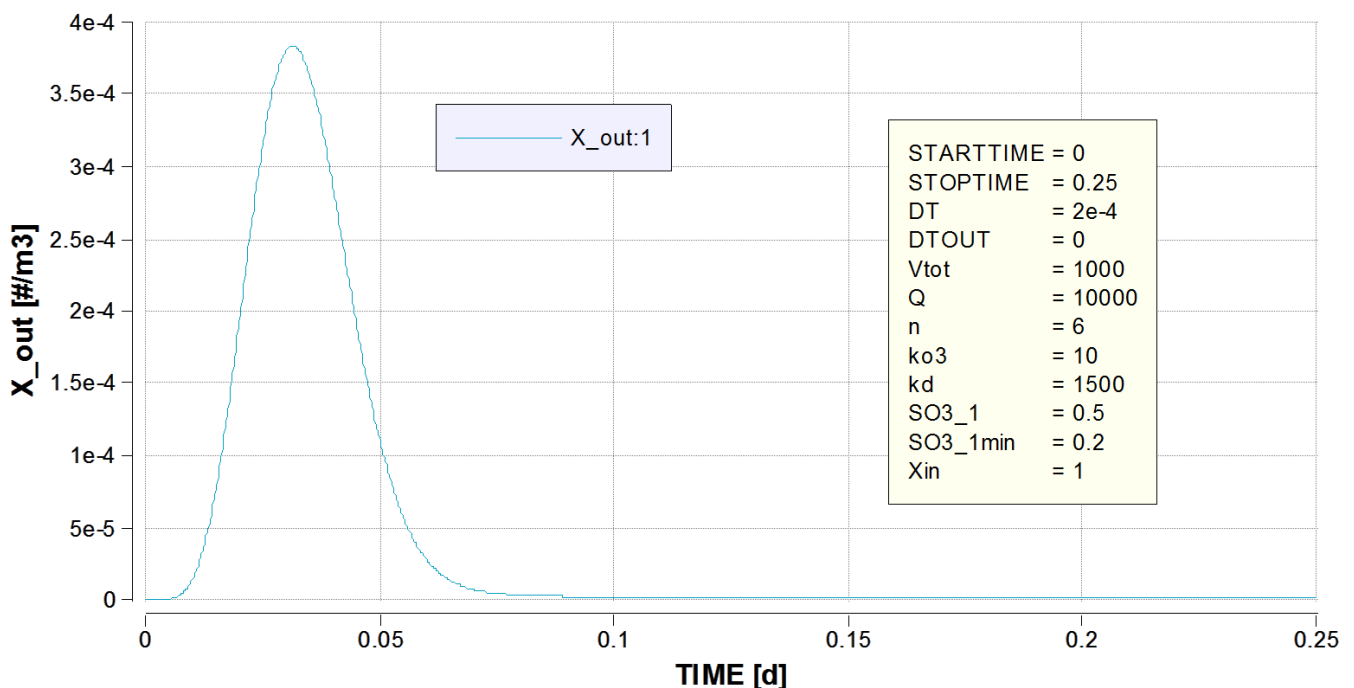


Figure 1: Steady state effluent concentration of the bacteria, for $n = 6$ reactors in series.

By means of the Gaussian error propagation, the standard error $\sigma_{X_{out}}$ of the effluent bacteria concentration resulting from the model parameters p_j can be computed as follows:

$$\sigma_{X_{out}} = \sqrt{\sum_{j=1}^k \sigma_{p_j}^2 * \left(\frac{\partial X_{out}}{\partial p_j}\right)^2}$$

The partial derivatives $\frac{\partial X_{out}}{\partial p_j}$ can be determined in BM in a sensitivity analysis (Parameters > Sensitivity), they correspond to the relative sensitivity of the state variable X_{out} :

$$\frac{\partial X_{out}}{\partial Q} = 4.64 * 10^{-10} \frac{\# * d}{m^6}$$

$$\frac{\partial X_{out}}{\partial k_{O_3}} = 2.50 * 10^{-7} \frac{\# * d}{m^3}$$

$$\frac{\partial X_{out}}{\partial k_D} = -4.74 * 10^{-9} \frac{\# * gO_3 * d}{m^6}$$

$$\frac{\partial X_{out}}{\partial S_{O_3,1}} = -1.42 * 10^{-5} \frac{\#}{gO_3}$$

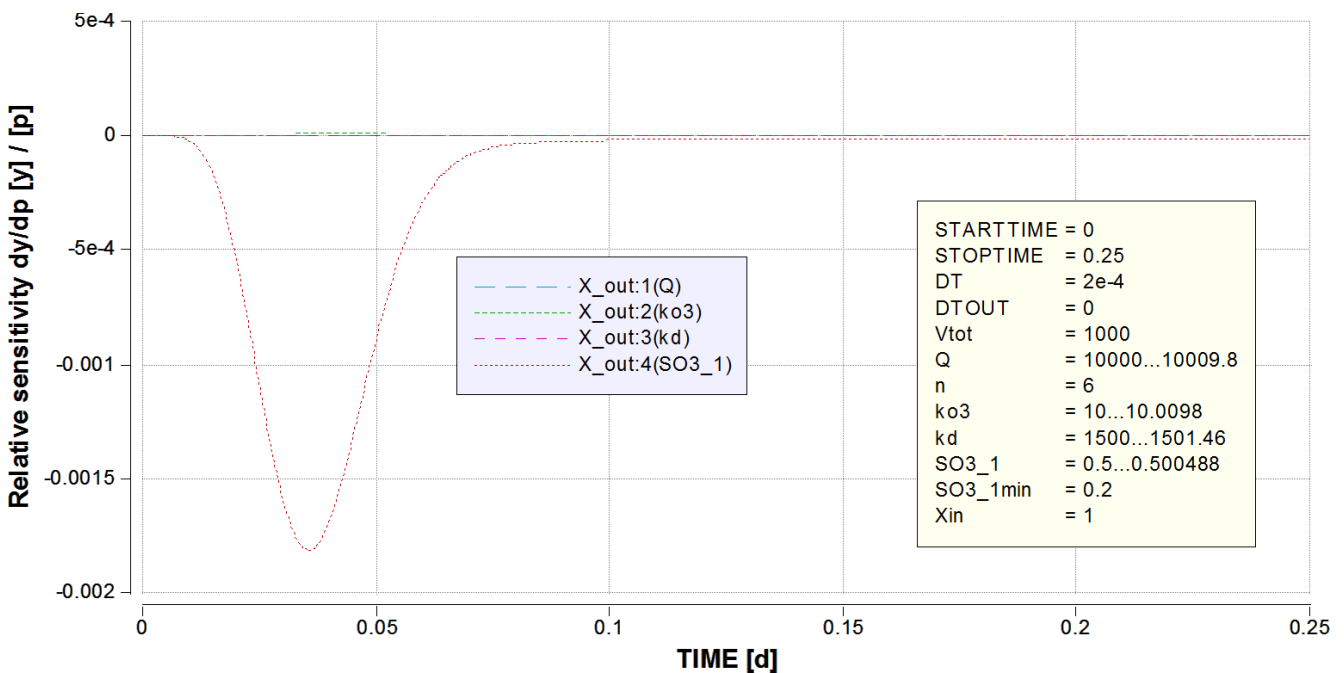


Figure 2: Partial derivatives of the state variable X_{out} relative to the parameters Q , k_{O_3} , k_D and $S_{O_3,1}$.

The standard error $\sigma_{X_{out}}$ is thus:

$$\sigma_{X_{out}}^2 = \left(500 \frac{m^3}{d} * 4.64 * 10^{-10} \frac{\# * d^2}{m^6} + \left(2 d^{-1} * 2.50 * 10^{-7} \frac{\# * d}{m^3} \right)^2 \right.$$

$$\left. + \left(150 \frac{m^3}{gO_3 * d} * -4.74 * 10^{-9} \frac{\# * gO_3 * d}{m^6} \right)^2 + \left(0.05 * -1.42 * 10^{-5} \frac{\#}{gO_3} \right)^2 \right.$$

$$\rightarrow \sigma_{X_{out}} = \sqrt{\sigma_{X_{out}}^2} = 1.15 * 10^{-6} \frac{\#}{m^3}$$

The 95% confidence interval for the effluent bacteria concentration and fraction, respectively, is the following:

$$X_{out,95\%} = \mu \pm 2 * \sigma_{Xout} = 1.33 * 10^{-6} \pm 2.30 * 10^{-6} \frac{\#}{m^3} = 0.000133\% \pm 0.000230\%$$

The 95% confidence interval reaches strongly into the negative. This indicates, that the distribution of the effluent concentrations is skewed, and thus definitively not normal.

MC simulation:

In BM, the error propagation calculation by means of a MC simulation can be done by using the function *Batch runs* (Parameters > Batch runs > Choose no parameter, Mode: Compute Mean ± SD).

The 95% confidence interval for the effluent bacteria concentration and fraction, respectively, is shown in Figure 3 and amounts to (with $\sigma_{Xout} = 2.0 * 10^{-6} \# / m^3$):

$$X_{out,95\%} = \mu \pm 2 * \sigma_{Xout} = 2.0 * 10^{-6} \pm 4.0 * 10^{-6} \frac{\#}{m^3} = 0.00020\% \pm 0.00048\%$$

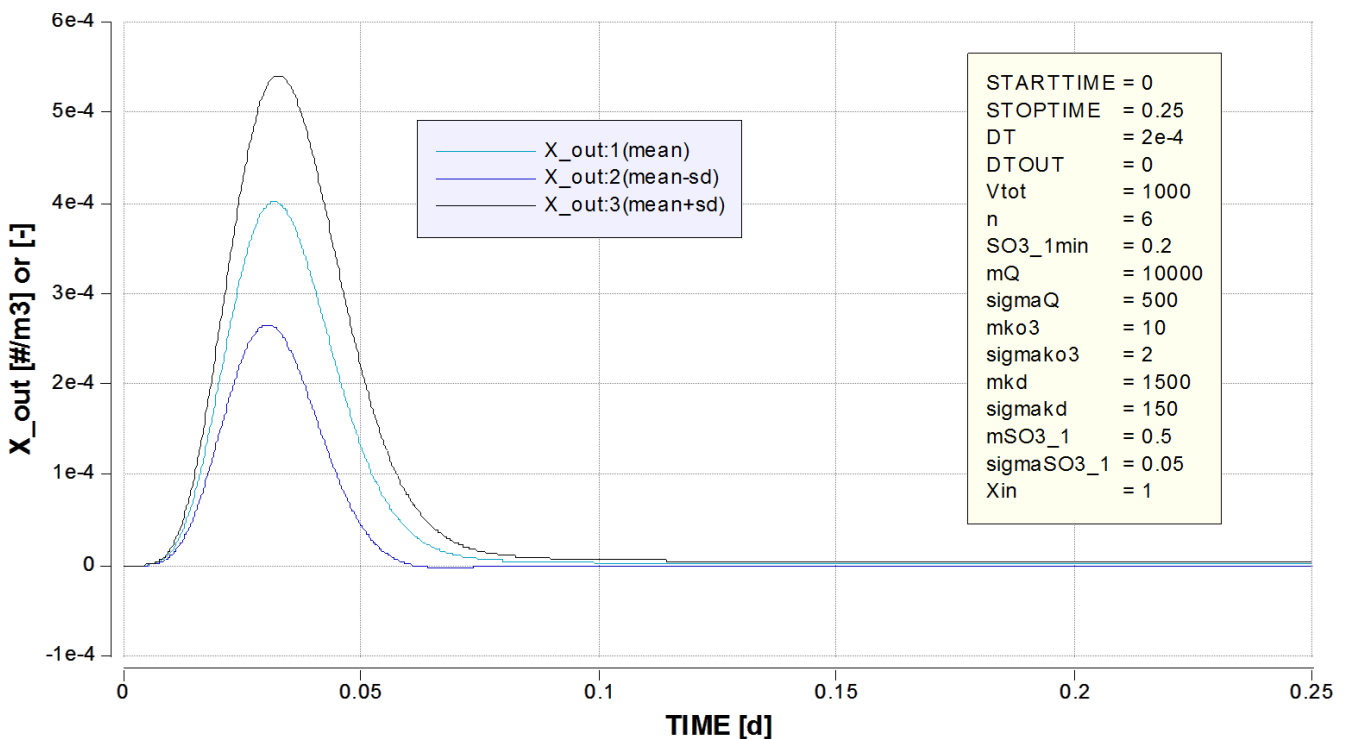


Figure 3: 95% confidence interval of the effluent bacteria concentration (fraction) determined by MC simulation.

It should be noted that the exact results for the confidence interval change for each new MC simulation, since the initial parameter values in BM are randomly chosen within the range of the indicated normal distribution.

It can be seen that the standard error in the MC simulation is twice as much as the one in the Gaussian error propagation.

Gaussian error propagation assumes a linearized model (e.g. normal distribution), whereas MC simulation can also deal with skewed distributions (the distribution of X_{out} is in fact skewed, therefore MC simulation is recommended).

2. Resulting uncertainty including uncertainty from hydraulic model

If additionally the uncertainty stemming from the hydraulic model is considered, the parameters V_{tot} (total volume) and n (number of reactors in series) have to be analysed, too. Here a Gaussian error propagation is not calculated, because the partial derivative of X_{out} relative to n , which is an integer, does not make much sense.

MC simulation:

The 95% confidence interval for the effluent bacteria concentration and fraction, respectively, is shown in Figure 5 and amounts to (with $\sigma_{X_{out}} = 1.9 \cdot 10^{-5} \text{ \#/m}^3$):

$$X_{out,95\%} = \mu \pm 2 * \sigma_{X_{out}} = 1.1 * 10^{-5} \pm 3.8 * 10^{-5} \frac{\#}{m^3} = 0.0011\% \pm 0.0038\%$$

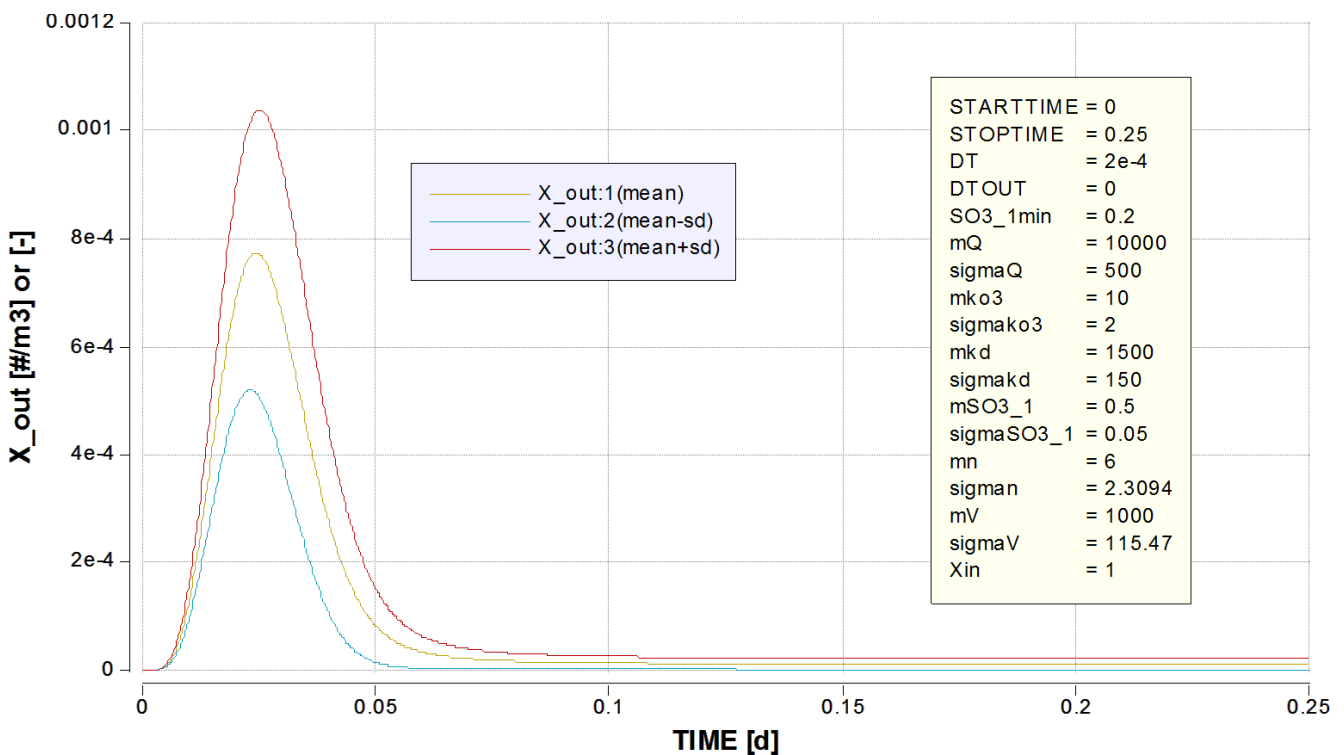


Figure 4: 95% confidence interval of the effluent bacteria concentration (fraction) determined by MC simulation, considering uncertainties from hydraulic model.

It can be concluded that the hydraulic model adds considerably to the overall uncertainty of X_{out} (see Table 1).

In the case of the Gaussian error propagation, the additional uncertainty from the hydraulic model leads to an almost doubled standard error for X_{out} . As for the MC simulation, both the mean and standard error of X_{out} increase roughly by a factor 10 (however, please note that this factor varies as well greatly between different MC simulations).

Table 1: Summary of the resulting uncertainty for X_{out} .

Error propagation model	95% confidence interval: $\mu_{X_{out}} + 2 * \sigma_{X_{out}}$ [# / m ³] or [-]	
	Neglecting uncertainty from hydraulic model	Considering uncertainty from hydraulic model
Gaussian error propagation	$1.33 * 10^{-6} \pm 2.30 * 10^{-6}$	---
MC simulation	$2.0 * 10^{-6} \pm 4.0 * 10^{-6}$	$1.1 * 10^{-5} \pm 3.8 * 10^{-5}$

In all three cases, the standard deviation of the results is larger than the expected value. This indicates that the distributions of the possible outcomes is skewed towards high values, a consequence of the non linearity of the model.

3. Guaranteed performance

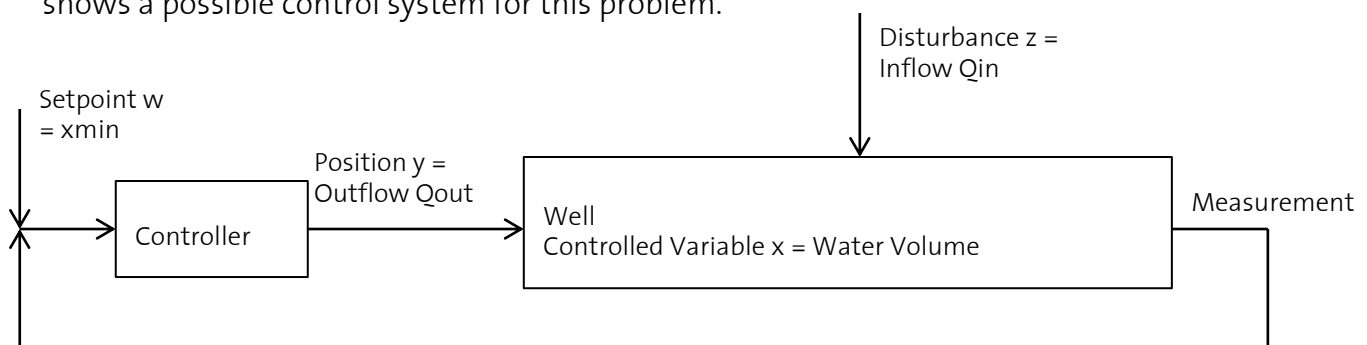
The performance that can be guaranteed to the owner of the plant is to be found at the lower end of the confidence interval. Maybe it would be best to communicate this uncertainty range by means of a worst case and a best case scenario.

In any case it is not sufficient to use two standard deviations (95%) for the definition of the confidence interval. Since the distribution of the possible outcomes is skewed, it is best to analyze the individual predictions themselves rather than their statistical properties.

Process Control, Two-Position Controller

1. System identification: controlled variable x , position y

The first step to design a control system is to define the system that one wants to control and identify the controlling variable or position y and the controlled variable x . The following sketch shows a possible control system for this problem.



The inflow into the pumping well is the disturbance z of the system. The volume in the well will change according to the disturbance and can be controlled by the outflow. The water volume in the well is the controlled variable and is measured (by a pressure or water level probe), so we have a feedback control. The measurement is compared to the setpoint, the minimum volume in the well, and the position y is set accordingly. As the pump can pump at $0.012\text{m}^3/\text{s}$ or be turned off, the two positions of the controller are those two values. The pump should be turned on again only after it has been off for 5min so the controller has to take this into account as well. In the real system it has to be taken care, that the well is big enough to receive 5min of maximum inflow ($x_{\min} + 3\text{m}^3$).

2. Time course and characteristic curve of the controller

Figure 1 shows the characteristic curve of the controller (left) and the time course of the controlled variable x and the position y (right).

The value x_{\max} is not a constant value. x_{\min} determines when the pump should be turned on and off. But as the pump should only be turned on again 5min after it has been turned off, the controller has to wait before it changes its position to y_{\max} , resulting in different x_{\max} , depending on the varying inflow.

The time course of the volume in the well, the controlled variable, has a zigzag pattern. The slopes change depending on the inflow and they are not straight lines, as painted here, as the inflow changes every second. The position has two values, either on or off and the off periods last at least 5min.

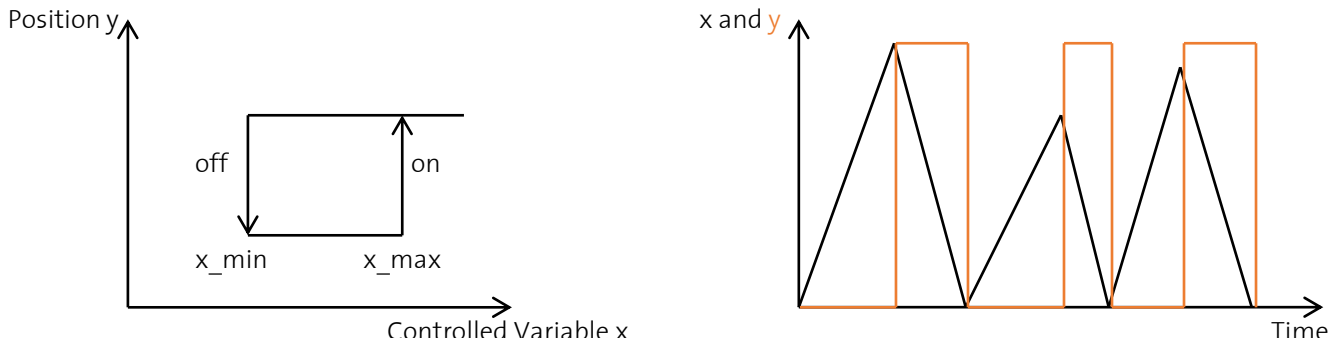


Figure 1: Characteristic Curve (left) and Time Course of Controlled Variable x and Position y (right)

3. Simulation in BM

The controller can be simulated in BM with the code shown below. The graph in figure 2 shows the result of a simulation over one hour starting with an empty well. The variable *count* ensures that the pump is off for at least 5min. Every second the position is at y_{\min} it adds +1 to the variable *count*. Only when *count* is equal or bigger than 300 can the position change to y_{\max} and the pump is turned on.

```

METHOD RK4

STARTTIME = 0
STOPTIME = 3600 ;1hr in s
DT = 1

;Incoming waste water into the pumping well, m3/s
init Qin = 0.005
next Qin = 0.99*Qin + random(-0.00035, 0.00045, 1)

;Qout = 0.012 ; Max. capacity of the pump, m3/s

;==MASS BALANCE==
init V = 0
d/dt(V) = Qin - Qout ; Mass balance of water volume in pumping well, m3

;==TWO-POSITION CONTROLLER==
x = V ; Controlled variable x
Qout = y ; Resulting position y

y_min = 0 ; No pumping, m3/s
y_max = 0.012 ; Max. capacity of the pump, m3/s

x_min = 0.012 ; Minimal water volume in pumping well, m3

Tt = 5*60 ; Delay time for pumping start signal, s
init count=0
next count=if y=y_min then count+1 else 0

init y = y_min
next y = if x < x_min then y_min else if (x > x_min and count>=Tt) then y_max else y

```

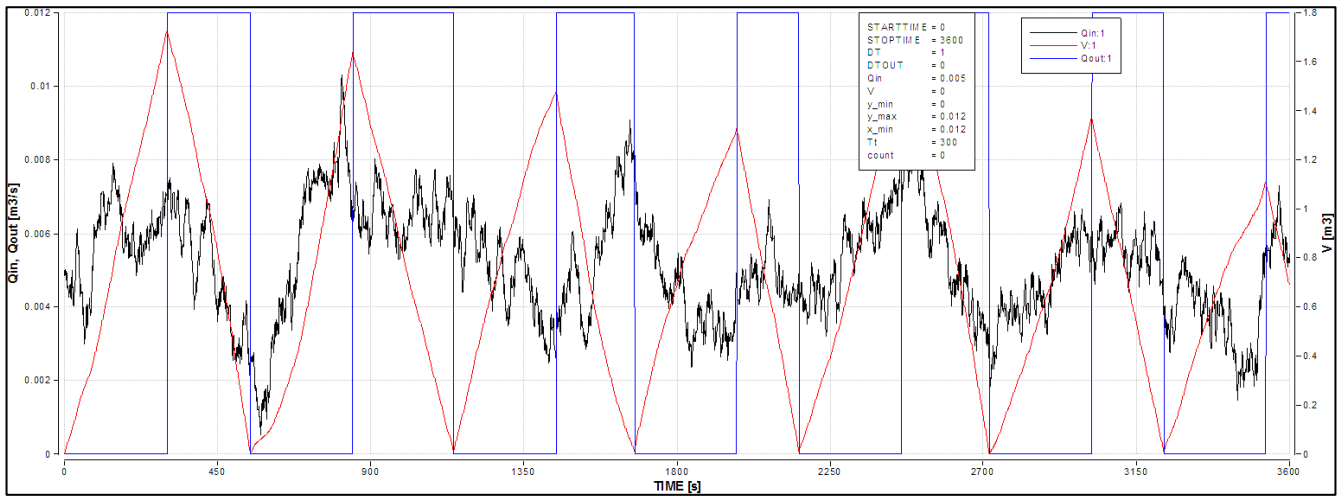



Figure 2: Simulation of the implemented controller over one hour

Process control, PID Controller

1. Plant at steady state

In a first step, the plant is modelled with a constant influent ($Q = 100 \text{ m}^3/\text{d}$, $S_{\text{COD},\text{in}} = 3000 \text{ gCOD}/\text{m}^3$ and $Q_P = 0.08 \text{ m}^3/\text{d}$). The steady state concentrations for the organic substrate, the phosphorus and the heterotrophic bacteria are the following (see Figure 1):

$$S_{\text{COD}} = 1.26 \text{ gCOD}/\text{m}^3$$

$$S_P = 4.01 \text{ gP}/\text{m}^3$$

$$X_H = 1797.81 \text{ gCOD}/\text{m}^3$$

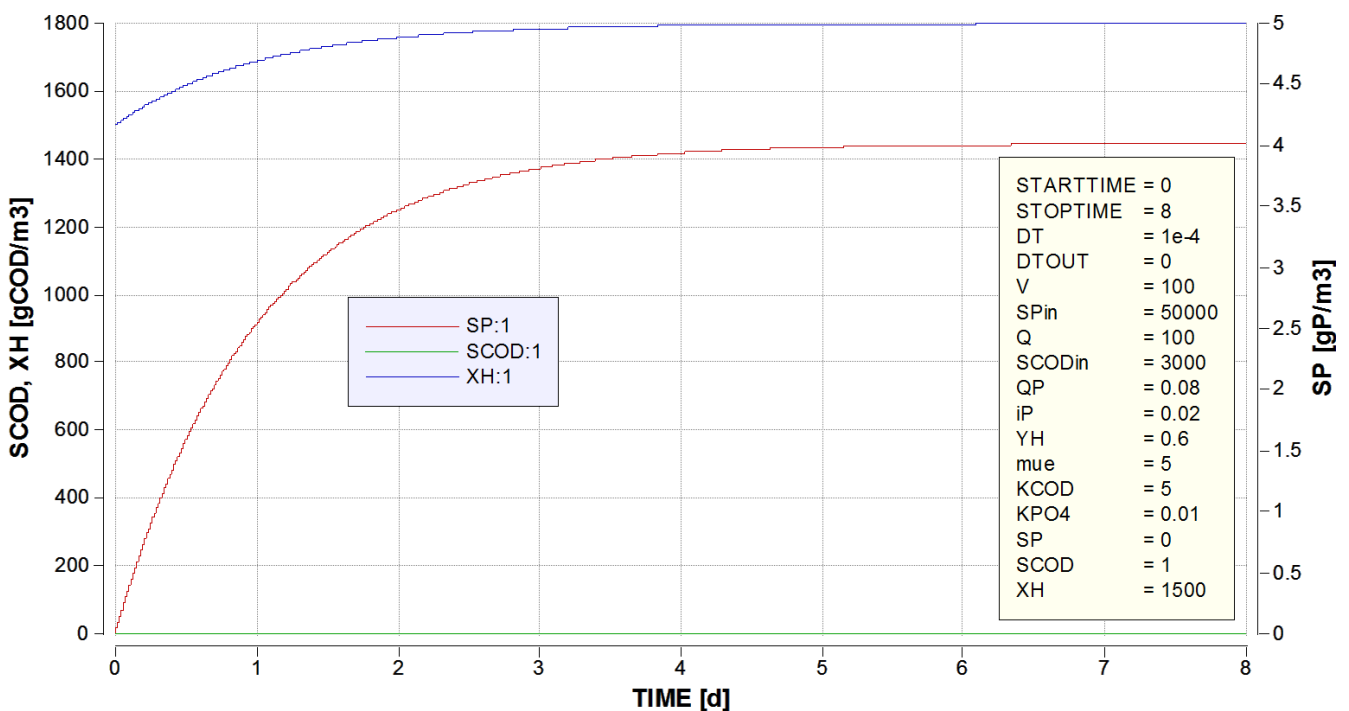


Figure 1: Steady state concentrations of organic substrate (S_{COD}), phosphorus (S_P) and heterotrophic bacteria (X_H) for a constant influent.

2. Implementation of PID controller at steady state

There are two different methods to identify the optimal parameters for the PID controller: either with an unstable controller or with a step input for Q_P , both implemented for constant influent conditions and later tested for a variable influent.

The controlled variable x is the effluent phosphorus concentration and the position is Q_P .

2.1 Method: Unstable controller, procedure by Ziegler and Nichols (1942)

P controller (with $K_I = 0$ and $K_D = 0$):

First, the resting position y_0 is determined by minimizing the offset e with the help of the function *Optimize*(expression "chi_2"). Make sure that you choose the appropriate range of values for y_0 (no negative values allowed). It becomes clear from looking at the system that the parameter K_P should be greater than 0, as a first guess 0.01 is chosen here. In Figure 2 it can be seen that for $y_0 = 0.0741$, the offset e is close to 0 gP/m^3 and S_P is close to the setpoint w (1 gP/m^3).

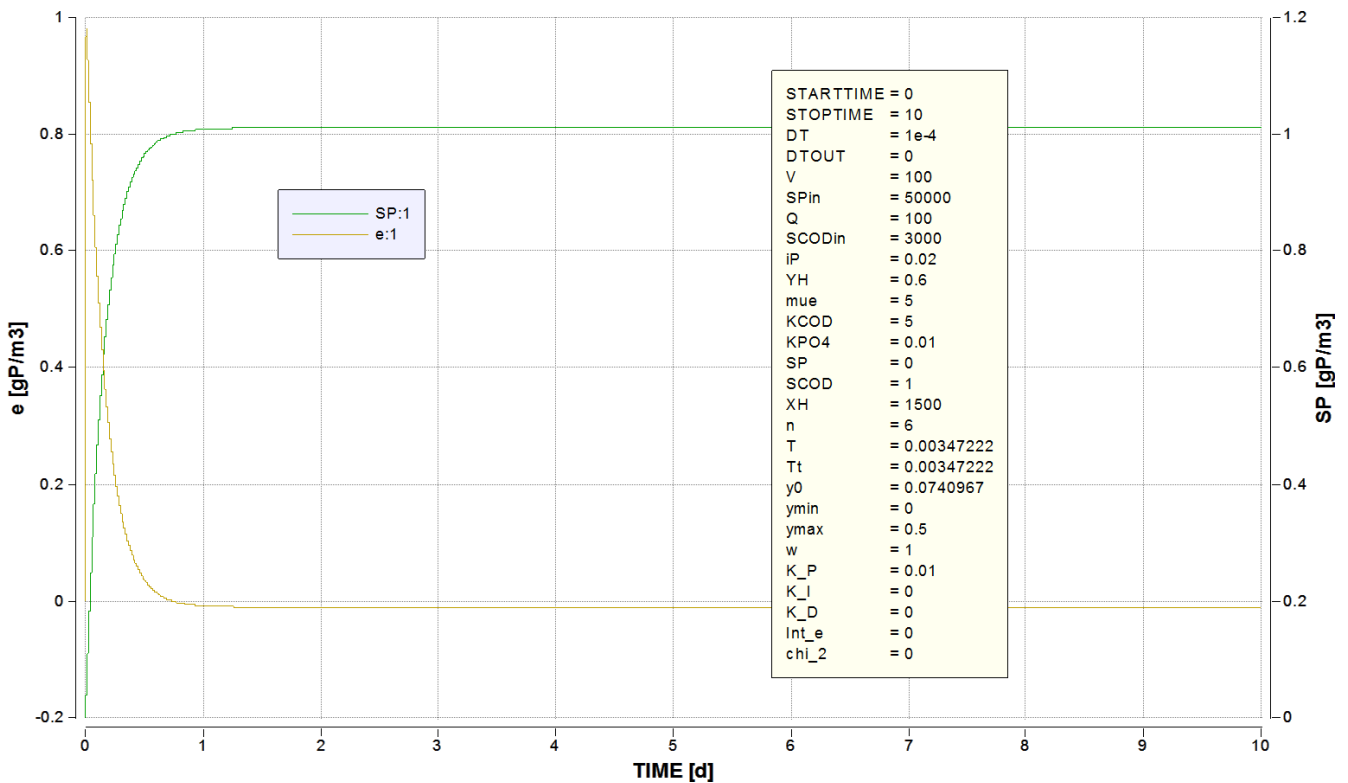


Figure 2: Minimizing the offset e by optimizing the parameter y_0 (for $K_P = 0.01$).

In a second step, the parameter K_P has to be determined. The crucial step is to determine $K_{P,crit}$ - the value of K_P at which the effluent phosphorus concentration S_P starts to oscillate. This happens for $K_P = 0.471 = K_{P,crit}$ (see Figure 3).

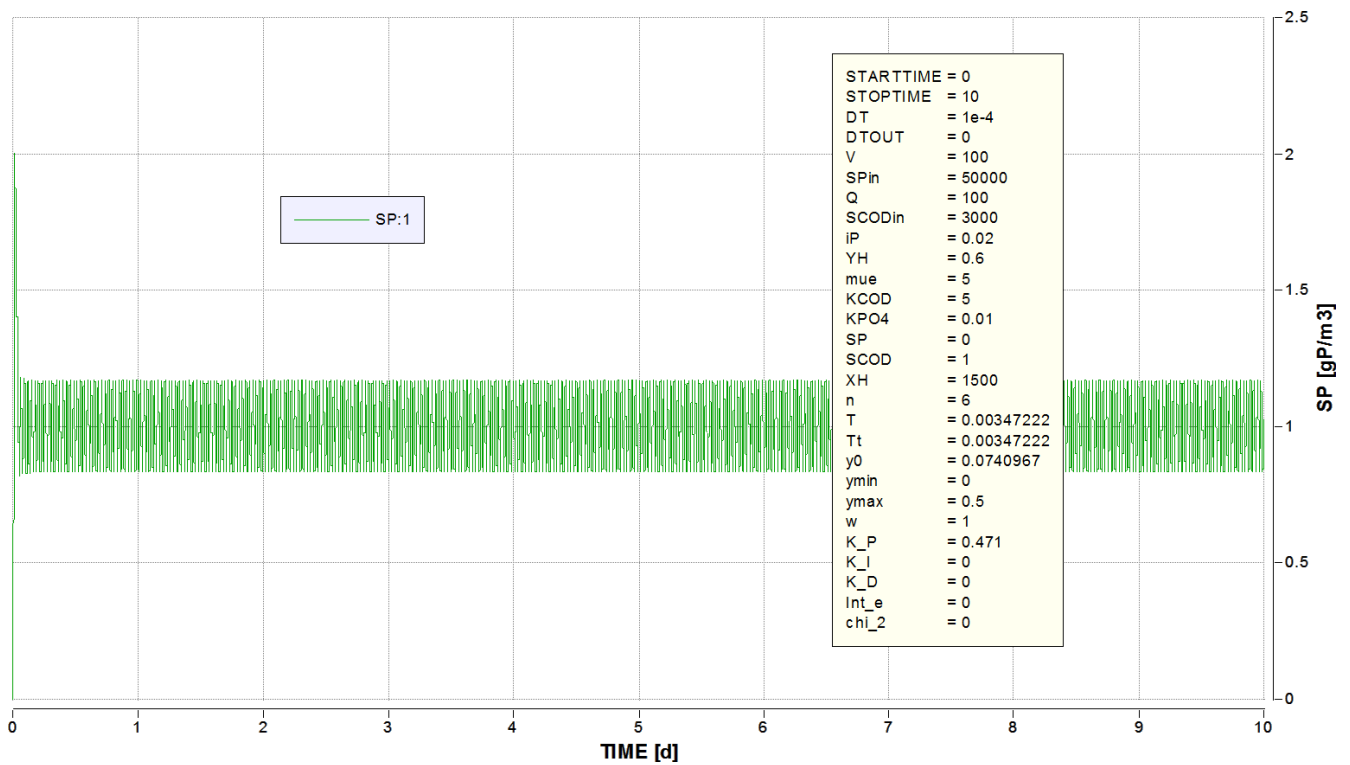


Figure 3: Determination of $K_{P,crit}$ where SP starts to oscillate.

According to the procedure by Ziegler and Nichols (see Gujer, Table 13.4), we would choose $K_P = 0.5 * K_{P,crit} = 0.2355$ for the operation of the P controller.

PI controller (with $K_D = 0$):

First, the period of the oscillation of the instable control loop, T_{crit} , has to be determined (see Figure 4), then K_P and K_I can be calculated as follows:

$$T_{crit} = (1.0465 \text{ d} - 1.0185 \text{ d}) = 0.028 \text{ d}$$

$$K_P = 0.45 * K_{P,crit} = 0.45 * 0.471 = 0.2120$$

$$K_I = \frac{K_P}{0.83 * T_{crit}} = \frac{0.2120}{0.83 * 0.028} = 9.120$$

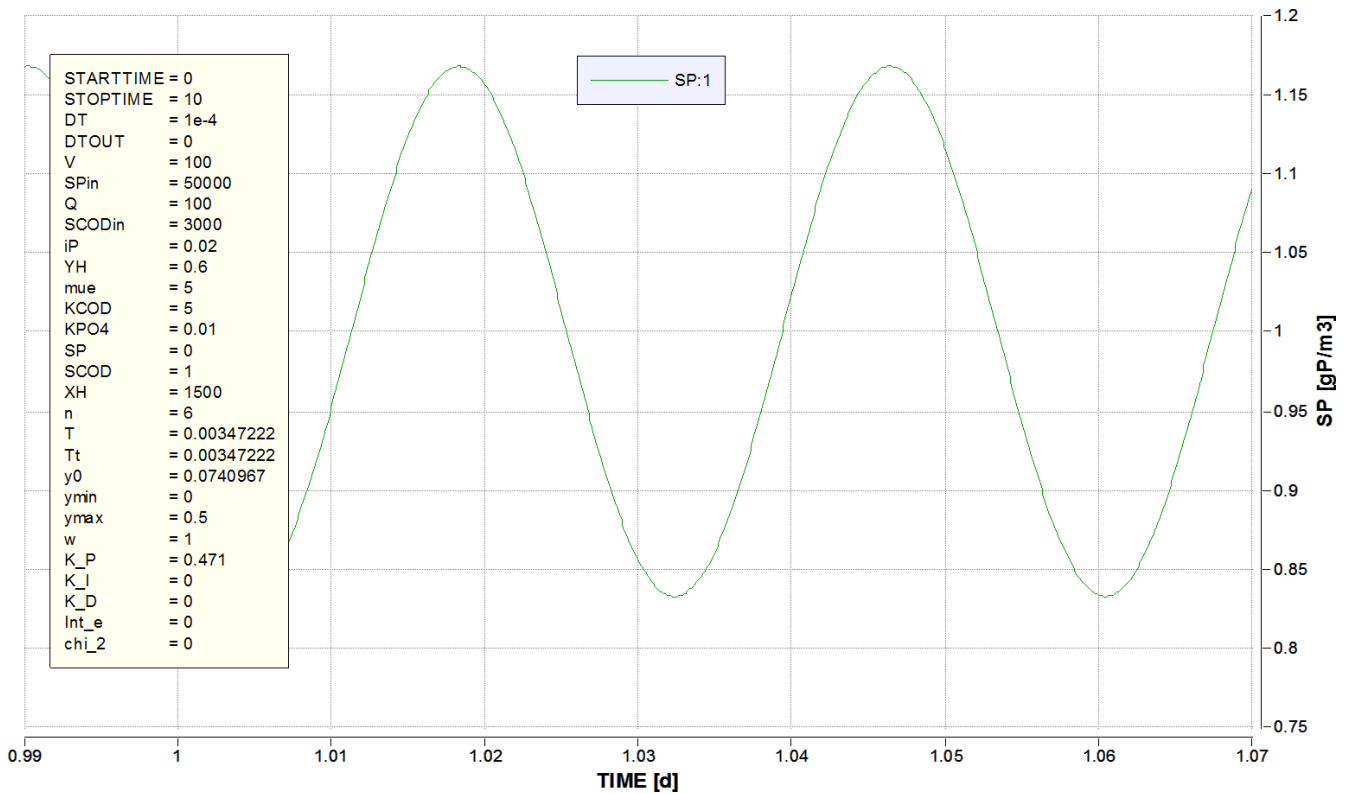


Figure 4: Determination of T_{crit} (period of the oscillation), for $K_{P,crit} = 0.471$.

PID controller:

$$K_P = 0.6 * K_{P,crit} = 0.6 * 0.471 = 0.2826$$

$$K_I = \frac{K_P}{0.5 * T_{crit}} = \frac{0.2826}{0.5 * 0.028} = 20.186$$

$$K_D = 0.125 * K_P * T_{crit} = 0.125 * 0.2826 * 0.028 = 9.891 * 10^{-4}$$

In Figure 5 it can be seen that for a constant influent, the goals of reaching an effluent phosphorus concentration of 1 gP/m³ and a minimal offset e can be achieved with this PID controller. However, as one can see in Table 1, for a constant influent, already the P controller would be sufficient to meet the requirements.

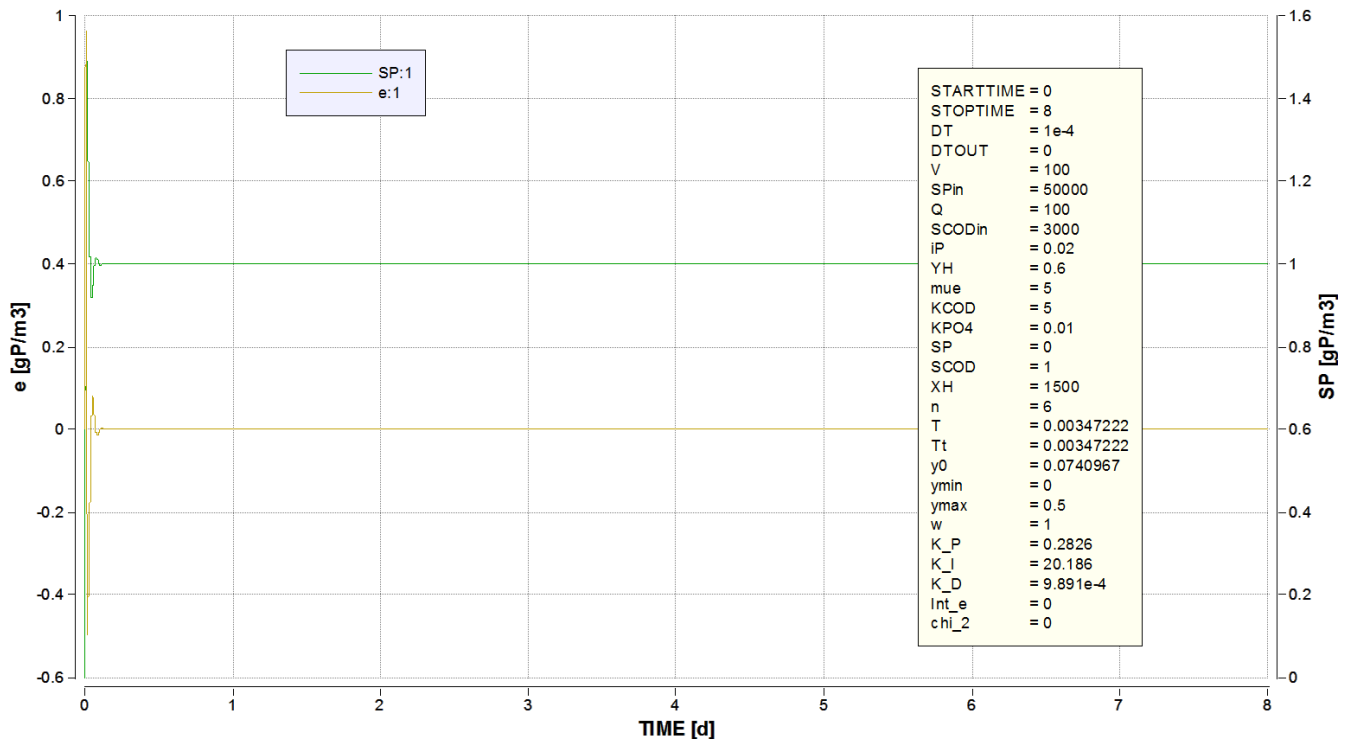


Figure 5: Constant influent: Resulting offset e and effluent phosphorus concentration S_P for the PID controller with the parameter values $K_P = 0.2826$, $K_I = 20.186$ and $K_D = 9.891 \cdot 10^{-14}$.

Table 1: Method: Unstable controller. Summary of the plant performance (e , S_P) and the optimal parameter sets for the three controller types; for a constant influent.

Type of controller	Optimal parameter set (according to Ziegler and Nichols, 1942)	Effluent phosphorus concentration S_P [gP/m ³]	Offset e [gP/m ³]
P controller	$K_P = 0.2355$	1.00053	$-5.29 \cdot 10^{-4}$
PI controller	$K_P = 0.2120$ $K_I = 9.120$	1.00	$-3.46 \cdot 10^{-14}$
PID controller	$K_P = 0.2826$ $K_I = 20.186$ $K_D = 9.891 \cdot 10^{-4}$	1.00	$-1.20 \cdot 10^{-14}$

2.2 Method: Step input for Q_P , procedure by Ziegler and Nichols (1942)

The simulation of a step response curve is another method to determine the parameter values for the PID controller.

P controller (with $K_I = 0$ and $K_D = 0$):

The simulation of a step change of Q_P (Δy) with inactive automatic controller allows to determine the size of the jump in the controlled variable S_P (Δx) and consequentially the proportionality coefficient $K_S = \Delta x / \Delta y$. Furthermore, the step response curve is used to determine the total delay time T_u and the transition period T_g .

With the help of Figure 6 and Figure 7, the relevant parameters can be estimated for a step change of Q_P of $\Delta y = 0.01 \text{ m}^3/\text{d}$:

$$T_u \approx 0.007 \text{ d} \approx 10 \text{ min}$$

$$T_g \approx 1.1 \text{ d} \approx 26.4 \text{ h}$$

$$\Delta x = 5.0 \text{ gP}/\text{m}^3$$

$$\rightarrow K_S = \frac{\Delta x}{\Delta y} = \frac{5.00}{0.01} = 500$$

According to Ziegler and Nichols, the value for K_P is then (see Gujer, Table 13.5):

$$K_P = \frac{T_g}{K_S * T_u} = \frac{1.1 \text{ d}}{500 * 0.007 \text{ d}} = 0.314$$

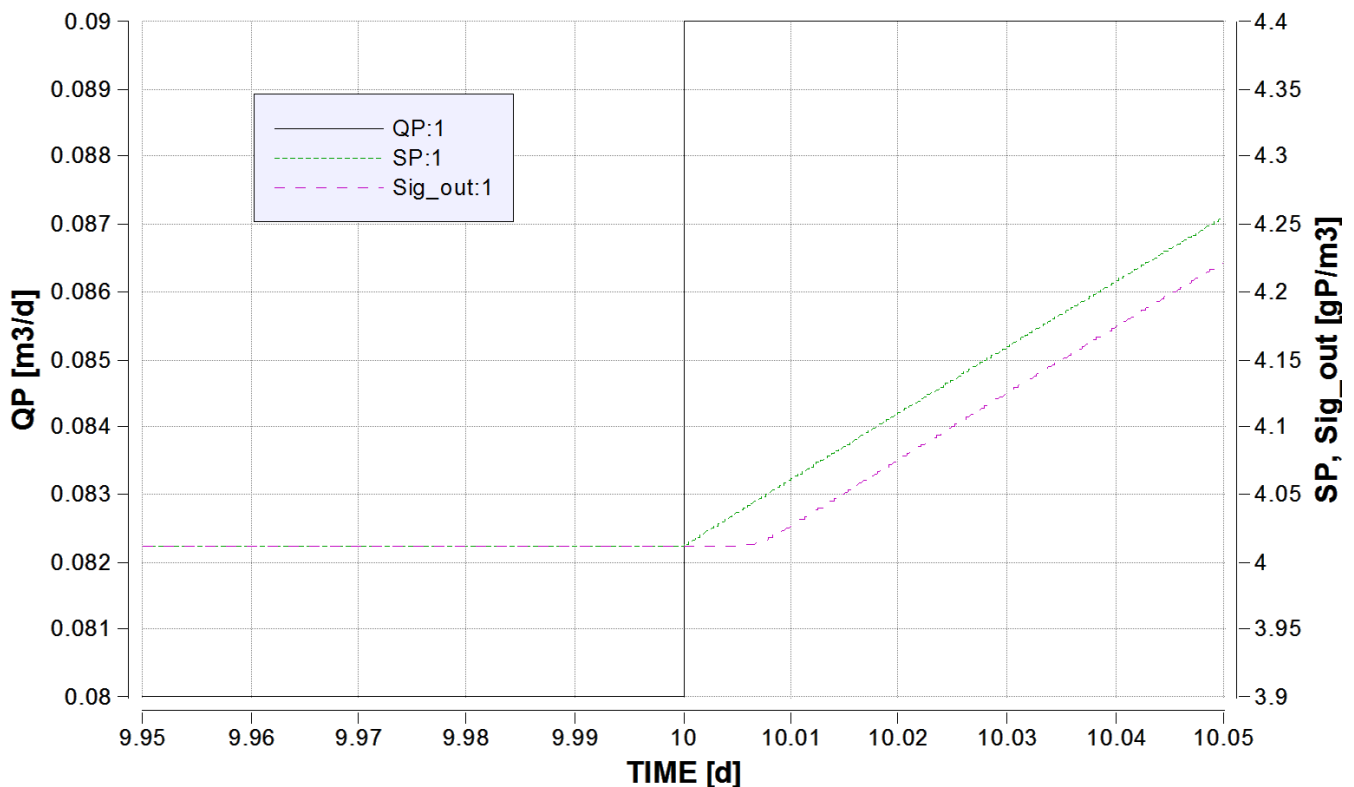


Figure 6: Simulation of a step change of the Q_P value: determination of T_u (dead time plus apparent dead time), which is the delay of the signal (Sig_out) compared to S_P .

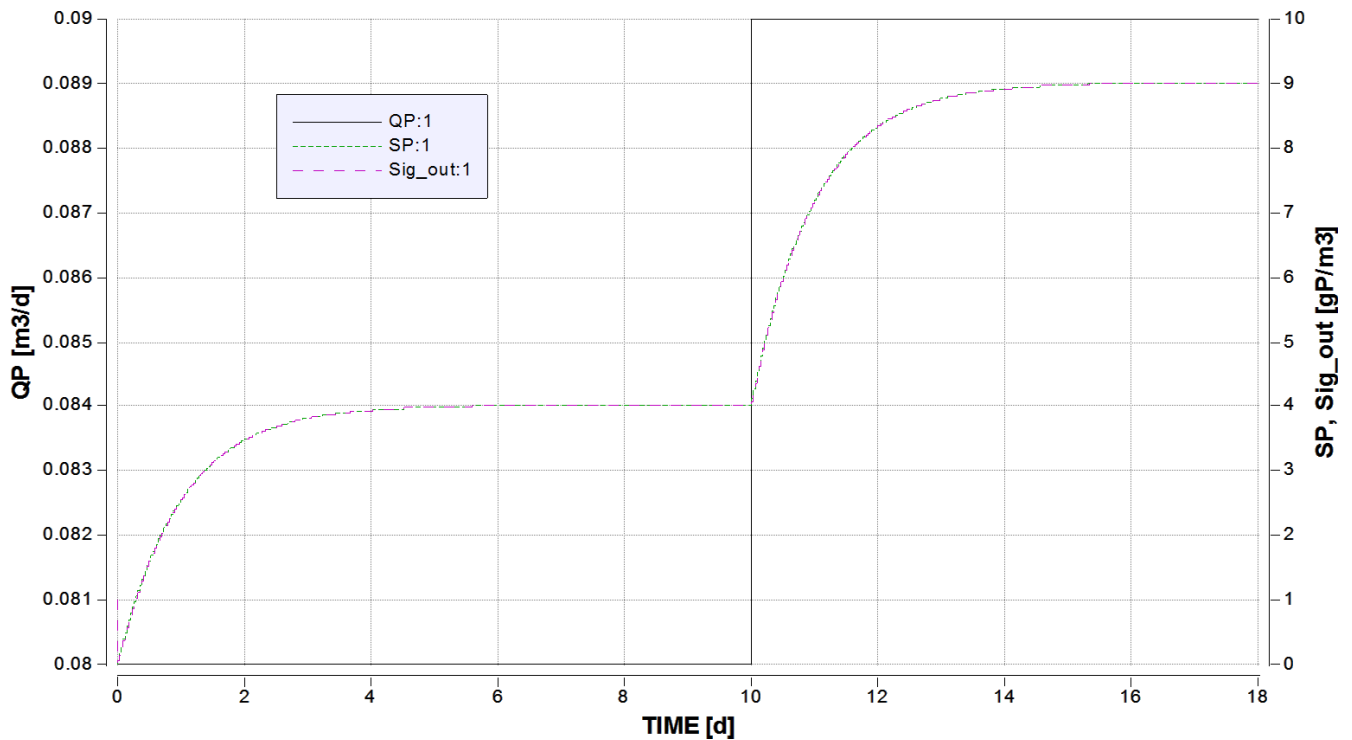


Figure 7: Simulation of a step change of the Q_p value: determination of T_g (transitory period) and Δx ($= \Delta \text{Sig_out}$).

PI controller (with $K_D = 0$):

$$K_P = 0.9 * \frac{T_g}{K_S * T_u} = 0.9 * \frac{1.1 \text{ d}}{500 * 0.007 \text{ d}} = 0.283$$

$$K_I = \frac{K_P}{3.3 * T_u} = \frac{0.283}{3.3 * 0.007} = 12.245$$

PID controller:

$$K_P = 1.2 * \frac{T_g}{K_S * T_u} = 1.2 * \frac{1.1 \text{ d}}{500 * 0.007 \text{ d}} = 0.377$$

$$K_I = \frac{K_P}{2.0 * T_u} = \frac{0.377}{2.0 * 0.007} = 26.939$$

$$K_D = 0.5 * K_P * T_u = 0.5 * 0.377 * 0.007 = 1.32 * 10^{-3}$$

When comparing the results of the two methods (Table 1 and Table 2), one can see that the parameter sets for the different controller types are different, however, the order of magnitude of the resulting plant performance (S_P , e) is very similar.

Table 2: Method: Step response curve. Summary of the plant performance (e , S_P) and the optimal parameter sets for the three controller types; for a constant influent.

Type of controller	Optimal parameter set (according to Ziegler and Nichols, 1942)	Effluent phosphorus concentration S_P [gP/m ³]	Offset e [gP/m ³]
P controller	$K_P = 0.314$	1.0004	$-3.98 \cdot 10^{-4}$
PI controller	$K_P = 0.283$ $K_I = 12.245$	1.00	$-2.55 \cdot 10^{-14}$
PID controller	$K_P = 0.377$ $K_I = 26.939$ $K_D = 1.32 \cdot 10^{-3}$	1.00	$-1.27 \cdot 10^{-14}$

3. Test of PID controller for variable influent

The plant performance for a variable influent without PID controller is shown in Figure 8:

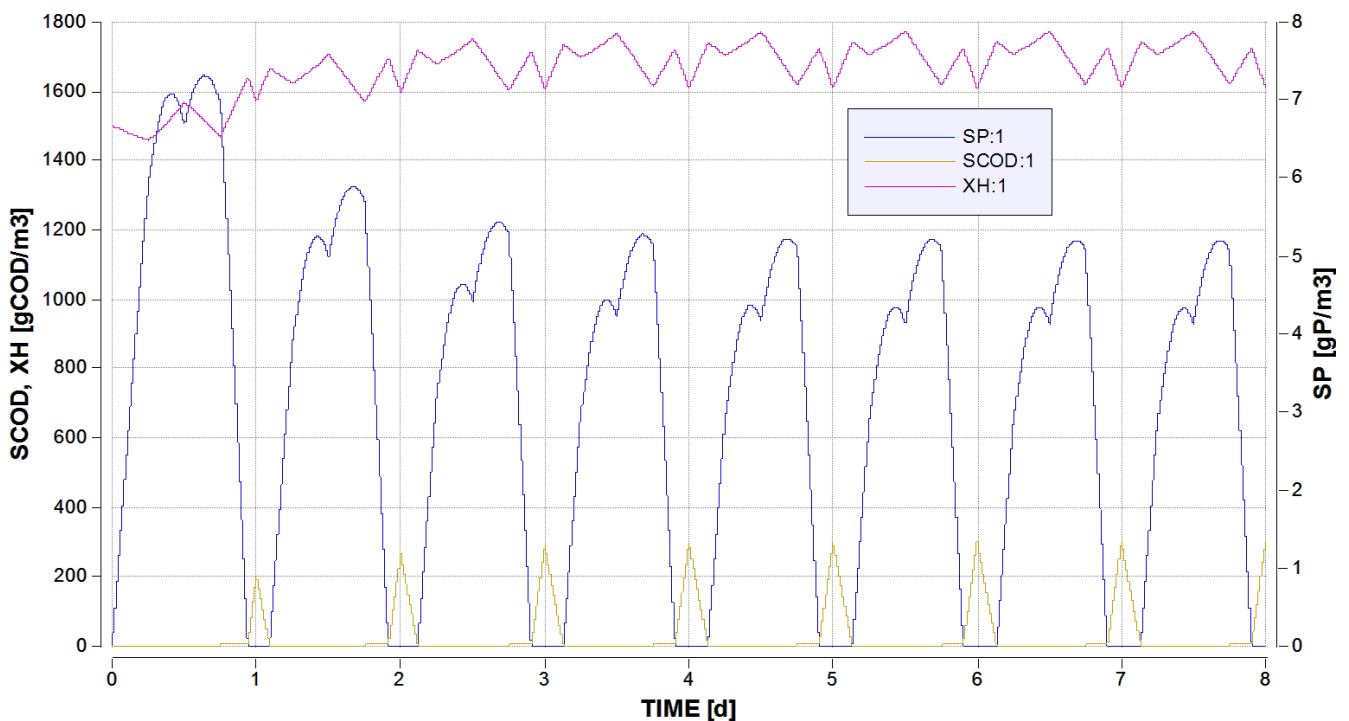


Figure 8: Varying concentrations of organic substrate (S_{COD}), phosphorus (S_P) and heterotrophic bacteria (X_H) for a variable influent (Q , $S_{COD,in}$) and $Q_P = 0.08 \text{ m}^3/\text{d} = \text{constant}$.

In Figure 9 it can be seen that the PID controller derived from the unstable controller can considerably decrease the range of fluctuations of the effluent phosphorus concentration. However, it cannot remove the fluctuations completely, especially when the peaks of Q and $S_{COD,in}$ overlap (at $t = 1\text{d}$, 2d , etc.).

The same deficiencies arise for the PID controller derived from the step response curve (see Figure 10). But the resulting plant performance is slightly better compared to the PID controller identified by the unstable controller.

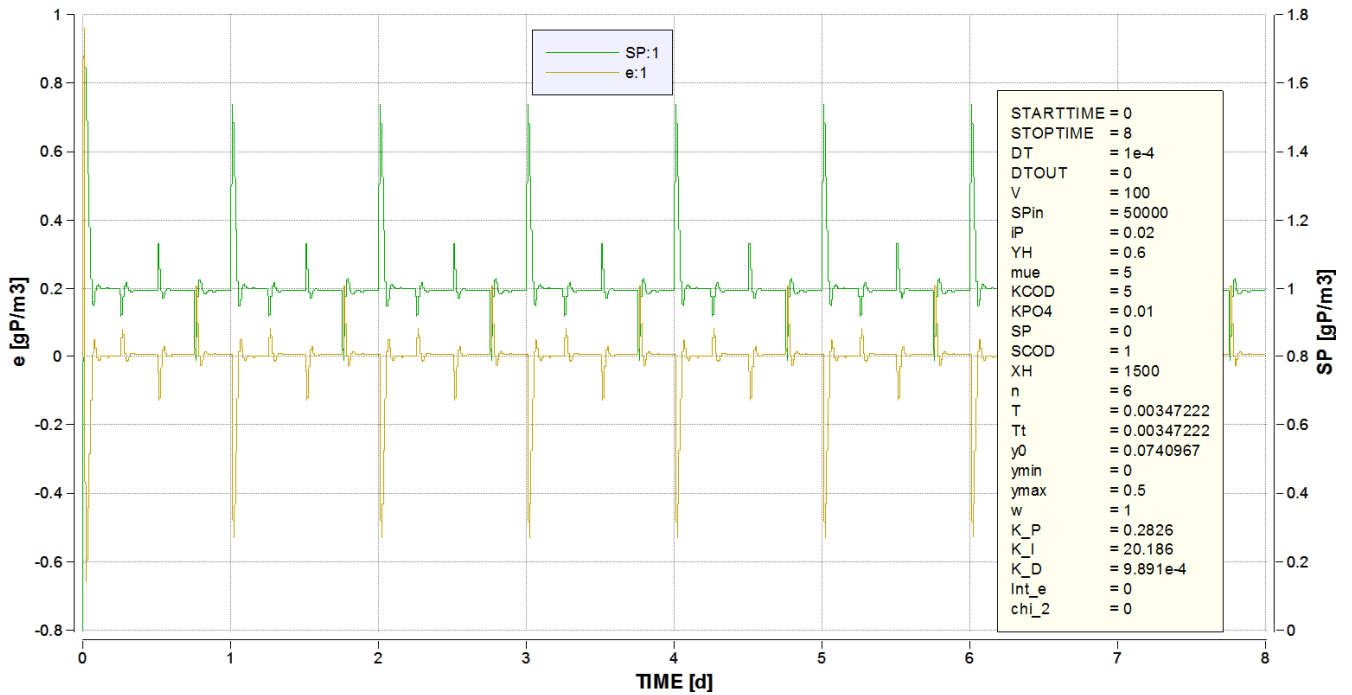


Figure 9: Variable influent (Q , $SCOD_{in}$): Resulting offset e and effluent phosphorus concentration SP for the PID controller derived from the instable controller.

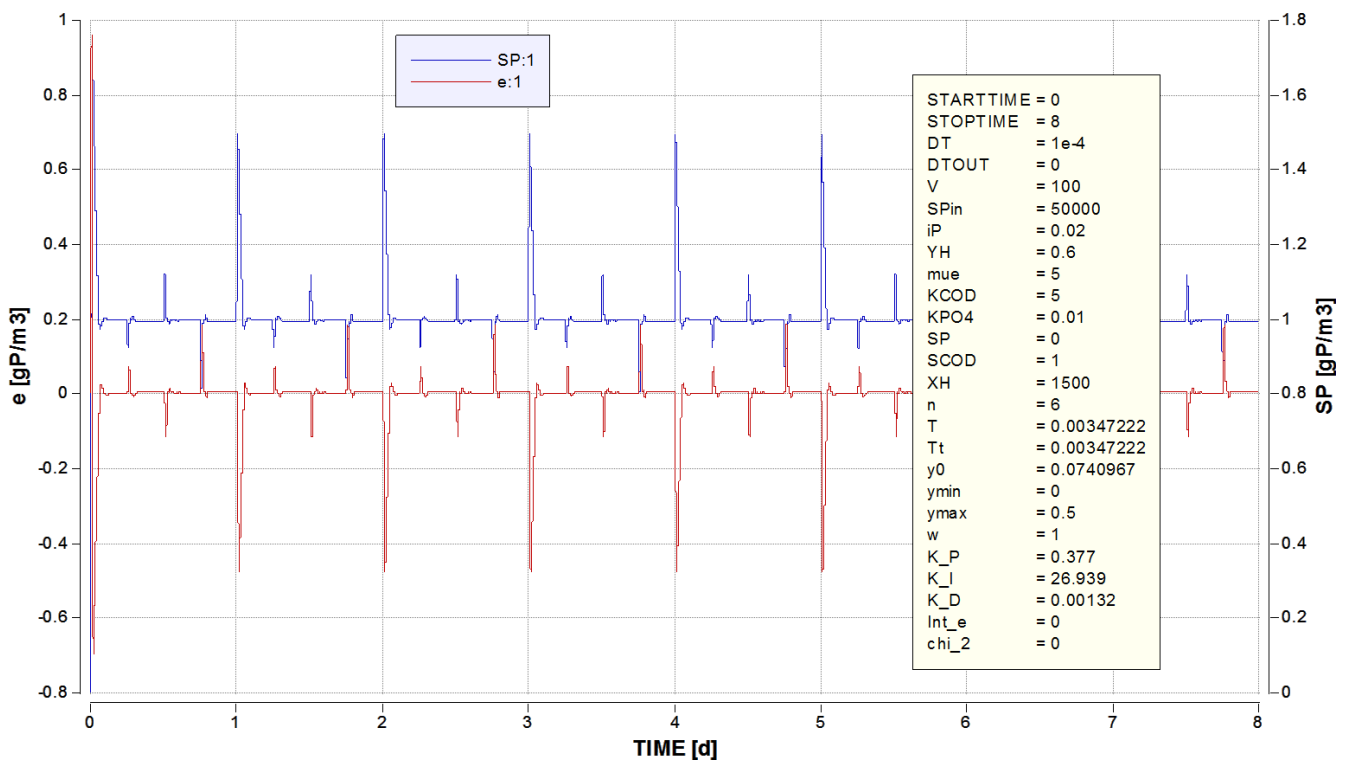


Figure 10: Variable influent (Q , $SCOD_{in}$): Resulting offset e and effluent phosphorus concentration SP for the PID controller derived from the step response curve.

4. Optimal parameter set

If the best parameters for the PID controller are identified by minimizing the root-mean-square offset, the following plant performance is obtained (for variable influent):

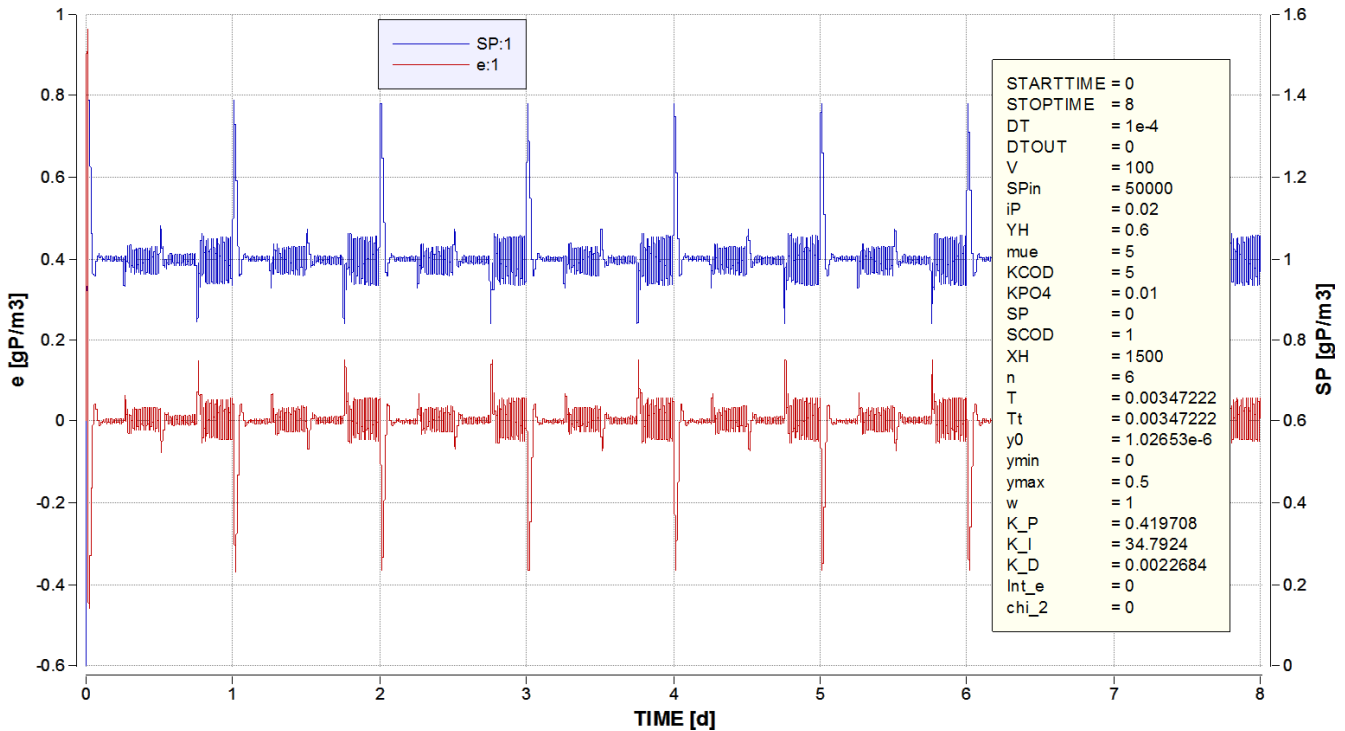


Figure 11: Variable influent (Q , $SCOD_{in}$): Resulting offset e and effluent phosphorus concentration S_P for the PID controller identified by minimizing the root-mean-square offset.

The parameter set of $y_0 = 1.02 \cdot 10^{-6}$, $K_P = 0.420$, $K_I = 34.792$ and $K_D = 0.0022$ leads to additional fluctuations in the effluent phosphorus concentration. The values obtained by simple optimization of the offset leads to too high parameter values which increase the instability of the system.

If the optimization of the parameters is done for constant influent and then tested for variable influent, the instability of the system is even higher and therefore this is not recommended.

Design under Uncertainty, Nitrification

1. Steady State

For the solution of this problem an equation system of mass balances for Ammonium and nitrifying biomass is necessary. To make this task easier a sketch of the activated sludge plant with all necessary flows and variables can be developed, as is shown below.

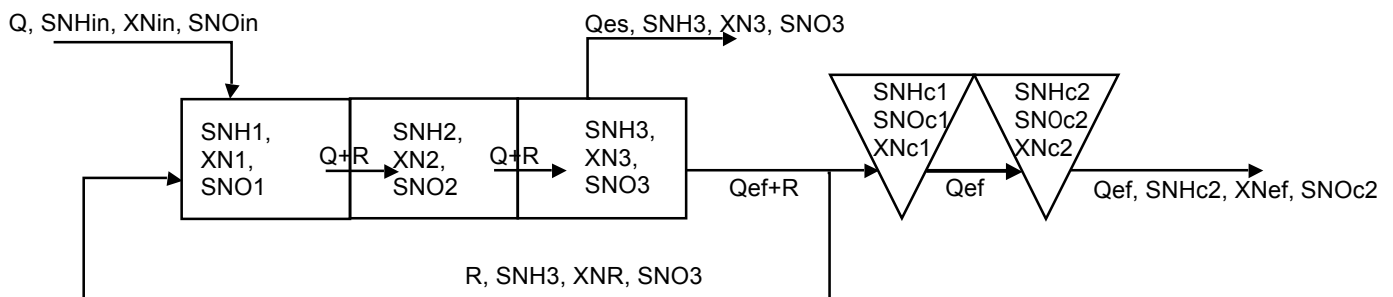


Figure 1: Sketch of the Treatment plant

The variables have the same names as in the BM-codes and also the clarifier has been split into two CSTRs. The concentrations of biomass in the two clarifiers are not really representative as they average over the whole clarifiers. Important is the concentration of biomass in the return sludge and the effluent. The biomass concentration in the return sludge can be computed by a mixing computation assuming that all biomass is in the return sludge and none in the effluent (ideal clarifier).

$$(Q_{ef} + R) \cdot XN_3 - R \cdot XNR = 0$$

$$XNR = \frac{Q_{ef} + R}{R} \cdot XN_3$$

The concentrations of Nitrate and Ammonium in the effluent are the same as in the second modelled clarifier, those in the return sludge the same as in the third reactor. The flow rate Q_{ef} equals the difference between the inflow Q and the excess sludge Q_{es} , which can be computed by an easy water mass balance around the third reactor. The inflow concentration of Nitrate SNO_{in} and nitrifying biomass XN_{in} are assumed to be zero, as well as the effluent concentration of particulates XN_{ef} .

By taking the return sludge out of the connection between reactors and clarifier, we don't need to keep track of the biomass in the clarifiers. The necessary mass balances for Ammonium and nitrifying biomass are then the following:

$$\text{Reactor 1: } \frac{dSNH1}{dt} = \frac{Q}{V} \cdot SNHin + \frac{R}{V} \cdot SNH3 - \frac{Q+R}{V} \cdot SNH1 - \frac{1}{Y_N} \cdot \mu_N \cdot \frac{SNH1}{K_{NH} + SNH1} \cdot XN1$$

$$\frac{dXN1}{dt} = \frac{R}{V} \cdot XNR - \frac{Q+R}{V} \cdot XN1 + \mu_N \cdot \frac{SNH1}{K_{NH} + SNH1} \cdot XN1 - b_N \cdot XN1$$

$$\text{Reactor 2: } \frac{dSNH2}{dt} = \frac{Q+R}{V} \cdot (SNH1 - SNH2) - \frac{1}{Y_N} \cdot \mu_N \cdot \frac{SNH2}{K_{NH} + SNH2} \cdot XN2$$

$$\frac{dXN2}{dt} = \frac{Q+R}{V} \cdot (XN1 - XN2) + \mu_N \cdot \frac{SNH2}{K_{NH} + SNH2} \cdot XN2 - b_N \cdot XN2$$

$$\text{Reactor 3: } \frac{dSNH3}{dt} = \frac{Q+R}{V} \cdot (SNH2 - SNH3) - \frac{1}{Y_N} \cdot \mu_N \cdot \frac{SNH3}{K_{NH} + SNH3} \cdot XN3$$

$$\frac{dXN3}{dt} = \frac{Q+R}{V} \cdot (XN2 - XN3) + \mu_N \cdot \frac{SNH3}{K_{NH} + SNH3} \cdot XN3 - b_N \cdot XN3$$

$$\text{Clarifier 1: } \frac{dSNHc1}{dt} = \frac{Q_{ef}}{V} \cdot (SNH3 - SNHc1)$$

$$\text{Clarifier 2: } \frac{dSNHc2}{dt} = \frac{Q_{ef}}{V} \cdot (SNHc1 - SNHc2)$$

With the following code the mass balances can be implemented in BM.

```

METHOD RK4

STARTTIME = 0
STOPTIME=100           ; days
DT = 1/24/60           ; time step in minutes

; FLOWS AND VOLUMES
Q=1000                 ; m3/d Inflow
R=1000                 ; m3/d Return sludge
Qes=60                 ; m3/d Excess sludge
Qef=Q-Qes              ; m3/d Effluent
V=200                  ; m3 aerated Vol. and Vol. of half a clarifier (modelled as 2CSTR)

; KINETIC PARAMETERS
my=0.3                 ; 1/d
K=1                    ; gN/m3
b=0.03                 ; 1/d
Y=0.24                 ; gCOD/gN
rr[1..3]=my*SNH[i]/(K+SNH[i])*XN[i]

; CONCENTRATIONS
SNHin=25               ; gN/m3
XNin=0                 ; gCOD/m3
XNR=(Qef+R)/R*XN[3]   ; gCOD/m3

```

```

;=====MASS BALANCES FOR AMMONIUM=====
init SNH[1..3]=0                                ;gN/m3
d/dt(SNH[1])=Q/V*SNHin+R/V*SNH[3]-(Q+R)/V*SNH[1]-1/Y*rr[1] ;1st reactor

d/dt(SNH[2..3])=(Q+R)/V*(SNH[i-1]-SNH[i])-1/Y*rr[i] ;2nd and 3rd reactor

init SNHc1=0                                     ;gN/m3
d/dt(SNHc1)=Qef/V*(SNH[3]-SNHc1)                ;1st CSTR of clarifier

init SNHc2=0                                     ;gN/m3
d/dt(SNHc2)=Qef/V*(SNHc1-SNHc2)                 ;2nd CSTR of clarifier

;=====MASS BALANCES FOR BIOMASS=====
init XN[1..3]=100                                ;gCOD/m3
d/dt(XN[1])=R/V*XNR-(Q+R)/V*XN[1]+rr[1]-b*XN[1] ;1st reactor

init XN[2..3]=100                                ;gCOD/m3
d/dt(XN[2..3])=(Q+R)/V*(XN[i-1]-XN[i])+rr[i]-b*XN[i] ;2nd and 3rd reactor

```

To implement steady state, the influent concentration of Ammonium is kept constant, and all the variables are represented by their expected values, so no uncertainty is considered. The effluent concentration of Ammonium (SNHc2) in steady state is 0.07gN/m³ and is reached after about 50 days of simulation.

2. Maximum daily Ammonium concentration in the effluent

The varying influent concentration can be added to the code as shown below. The hint in the book is used to find out the daily maximum concentration. Also the variable DTout has to be added to make sure that the daily maximum is found.

```

DTout=1                                           ;output every day

SNHin=25+15*sin(2*pi*time*f)                     ;gN/m3
f=1                                               ;1/d

;=====MAXIMUM AMMONIUM=====
init SMAX=0
next SMAX= if mod(time,1)<DT then 0 else max(SMAX, SNHc2)

```

The program then finds a maximum effluent concentration of 0.21gN/m³ which is still far below the requirements. Figure 2 shows the simulation over 5 days (to obtain these results you need to remove DTout).

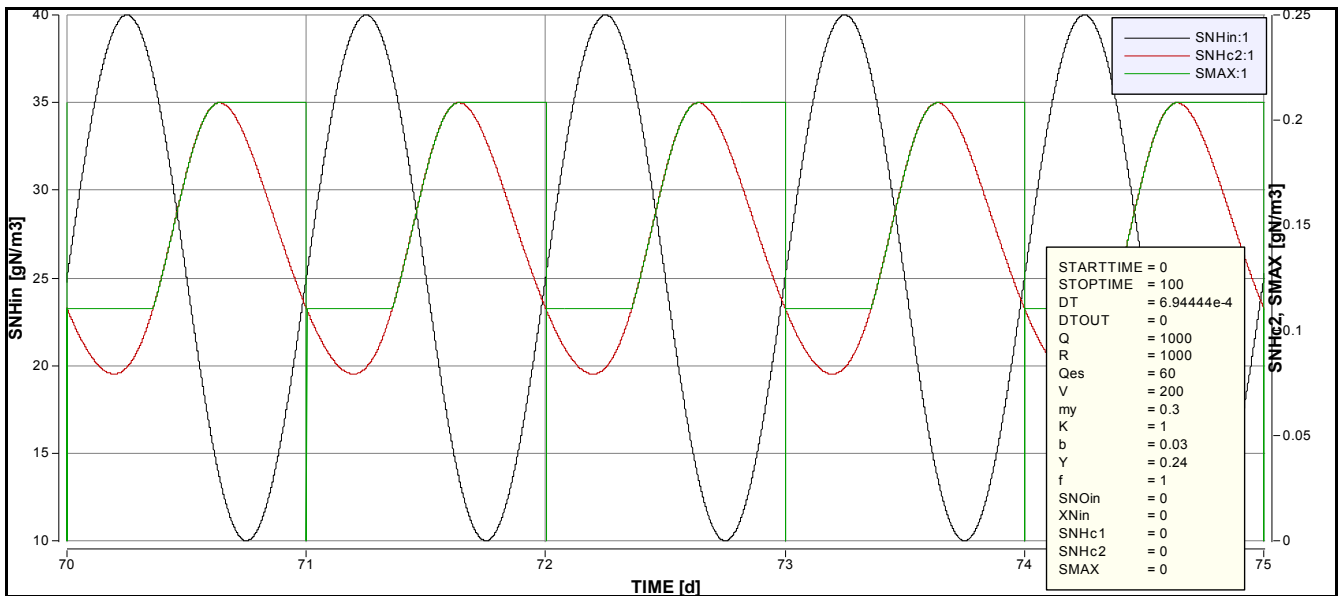


Figure 2: Simulation of Ammonium concentration in inflow and effluent and SMAX over 5days

3. Nitrate concentration in effluent

For this question more mass balances are needed. They are nearly the same as those for Ammonium. The only difference is that the influent concentration is zero and that the reaction rate is positive.

$$\text{Reactor 1: } \frac{dSNO1}{dt} = \frac{R}{V} \cdot SNO3 - \frac{Q+R}{V} \cdot SNO1 + \frac{1}{Y_N} \cdot \mu_N \cdot \frac{SNH1}{K_{NH} + SNH1} \cdot XN1$$

$$\text{Reactor 2: } \frac{dSNO2}{dt} = \frac{Q+R}{V} \cdot (SNO1 - SNO2) + \frac{1}{Y_N} \cdot \mu_N \cdot \frac{SNH2}{K_{NH} + SNH2} \cdot XN2$$

$$\text{Reactor 3: } \frac{dSNO3}{dt} = \frac{Q+R}{V} \cdot (SNO2 - SNO3) + \frac{1}{Y_N} \cdot \mu_N \cdot \frac{SNH3}{K_{NH} + SNH3} \cdot XN3$$

$$\text{Clarifier 1: } \frac{dSNOc1}{dt} = \frac{Q_{ef}}{V} \cdot (SNO3 - SNOc1)$$

$$\text{Clarifier 2: } \frac{dSNOc2}{dt} = \frac{Q_{ef}}{V} \cdot (SNOc1 - SNOc2)$$

The maximum concentration can be found in the same way as in the second part. This leads to the following addition in the BM code and to a maximum Nitrate concentration of 25.84gN/m³, which is lower than the maximal Input ammonium concentration of 40 gN m⁻³. This reduction is due to hydraulic dilution and not due to biological processes since neither nitrogen incorporation into biomass nor denitrification is considered in the model.

```

;=====MASS BALANCES FOR NITRATE=====
init SNO[1..3]=0.1 ;gN/m3
d/dt(SNO[1])=R/V*SNO[3]-(Q+R)/V*SNO[1]+1/Y*rr[1]

d/dt(SNO[2..3])=(Q+R)/V*(SNO[j-1]-SNO[j])+1/Y*rr[j]

init SNOc1=0.1 ;gN/m3
d/dt(SNOc1)=Qef/V*(SNO[3]-SNOc1)

init SNOc2=0.1 ;gN/m3
d/dt(SNOc2)=Qef/V*(SNOc1-SNOc2)

;=====MAXIMUM NITRATE=====
init SOMAX=0
next SOMAX= if mod(time,1)<DT then 0 else max(SOMAX, SNOc2)

```

4. Influence of secondary clarifier

When we filter out the maximum values of the effluent of the aerated reactors, not the effluent of the entire plant, we find that here the maximal Ammonium concentration is 0.38gN/m^3 instead of only 0.21gN/m^3 and the Nitrate concentration is 29.08gN/m^3 instead of 25.84gN/m^3 . This shows that the secondary clarifier reduces the extreme concentrations. As no reactions are simulated in the clarifier, this has to be due to the mixing (dispersion) that attenuates the oscillations of the Ammonium concentration in the influent.

```

;=====MAXIMUM NITRATE AFTER AERATION REACOTRS=====
init SOMAX=0
next SOMAX= if mod(time,1)<DT then 0 else max(SOMAX, SNO[3])

;=====MAXIMUM AMMONIUM AFTER AERATION REACOTRS =====
init SMAX=0
next SMAX= if mod(time,1)<DT then 0 else max(SMAX, SNH[3])

```

5. Risk of failure

Now we want to take the uncertainty of the different parameters into account. We use a MC simulation, thus the BM code has to be adapted and the parameters have to be chosen randomly for every run. Another addition can be made to count the days when the effluent concentration exceeds the requirements. For this we exclude the 50 first days before the plant reaches steady state. The code gives out the final value of exceedances at DTout. If an exceedance happens at more than 20% of the days in one simulation run, the design has failed. To calculate the risk of failure 1000 Batch runs (\rightarrow Parameters, Batch Runs, No Parameter) are conducted and then the number of runs, where the design has failed, is divided by 1000.

As 1000 runs are not enough to reach the real expected value, the percentage changes slightly. So 10 times 1000 runs were done and the average was taken. The result was a failure risk of about 19%.

METHOD RK4

```
STARTTIME = 0
STOPTIME=150           ; days
DT = 1/24/60           ; time step 1minute
DTout=150              ; output at end of simulation

;FLOWS AND VOLUMES
init Q=normal(1000,200) ;m3/d Inflow
next Q=if mod(time,1)<DT then normal(1000,200) else Q
R=1000                 ;m3/d Return sludge
init Qes=normal(60,6)  ;m3/d Excess sludge
next Qes=if mod(time,1)<DT then normal(60,6) else Qes
Qef=Q-Qes              ;m3/d Effluent
V=200                  ;m3 aerated Vol. and Vol. of half a clarifier (modelled as 2CSTR)

;KINETIC PARAMETERS
init my=random(0.2, 0.3) next my=my ;1/d
init K=random(0.5,2.5) next K=K ;gN/m3
init b=random(0.02,0.06) next b=b ;1/d
Y=0.24                ;gCOD/gN
r[1..3]=my*SNH[i]/(K+SNH[i])*XN1

;=====COUNT EXCEEDANCES=====
init SNMAX=0
next SNMAX= if mod(time,1)<DT then 0 else max(SNMAX, SNHc2)

init exc=0
next exc= if (mod(time,1)<DT and SNMAX>5 and time>50) then exc+1 else exc
```

Integrated Problem: Nitrification in a RBC

1. Verification of Flow Rate

The flow rate of the operator can be checked by comparing it to the flow rate, that can be calculated from the RTD. If we assume that the single reactors of the tertiary plant are closed to turbulence we can use equation 7.25 to calculate the flow.

$$\tau_m = \frac{V_{tot}}{Q} = \theta_h$$

$$Q = \frac{V_{tot}}{\tau_m} = 11982 \frac{m^3}{d} \approx 12000 \frac{m^3}{d}$$

The flow given by the operator underestimates the real value by about 20%. In the following calculation we will use a value of 12000 m³/d for the flow rate.

2. Cascade of CSTRs

To decide on a model for the secondary clarifier we first have to separate the RTD into the part resulting from the three RBC reactors and that of the clarifier. We can do this due to the additivity of the RTD characteristics. The hydraulic residence time of the three RBC tanks together can be calculated from their volume and the flow rate using equation 7.25.

$$\tau_{m,RCB} = \frac{V_{RCB}}{Q} = \theta_{h,RCB} = 0.0250d = 36 \text{ min}$$

With equation 7.26 we can then find out, which part of the standard deviation is caused by the RBC tanks, with n=3.

$$\sigma_{RCB}^2 = \frac{\theta_{h,RCB}^2}{n} = 0.000208d^2$$

$$\sigma_{RCB} = 0.0144d$$

The rest of the hydraulic residence time and the variance is caused by the clarifier. From this we can derive the number of reactors the clarifier should be modelled with.

$$\tau_{m,c} = \theta_c = \theta_{h,tot} - \theta_{h,RCB} = 0.1085d - 0.0250d = 0.0835d$$

$$\sigma_c^2 = \sigma_{tot}^2 - \sigma_{RCB}^2 = 0.003684d^2 - 0.000208d^2 = 0.003476d^2$$

$$\sigma_c = 0.0590d$$

$$n_c = \frac{\theta_{h,c}^2}{\sigma_c^2} = 2.01 \approx 2$$

The clarifier can be modelled using 2 CSTRs in series.

3. Stoichiometric and Composition Matrix

To find the missing stoichiometric coefficients $n_{j,i}$ we need the conservation laws of TOD and Nitrogen (eq. 5.10). Before we can use those we have to fill in the missing composition factors $i_{k,i}$. The composition factors of the conservative Nitrogen can easily be derived from the Nitrogen content in each species. For the TOD the example of Nitrite is given.

$$TOD_{NO_2} = \left[1 \cdot \left(-24 \frac{gTOD}{molN} \right) + 2 \cdot \left(-16 \frac{gTOD}{molO} \right) + 1 \cdot \left(8 \frac{gTOD}{mol, neg.char.} \right) \right] / 14 \frac{gN}{molNO_2} = -3.43 \frac{gTOD}{gN}$$

The conservation law can now be applied to both processes and both conservatives, resulting in four equations for the four unknown stoichiometric coefficients. Again one example is given, for the biomass in the Nitratation process.

$$\sum_i v_{j,i} \cdot i_{k,i} = \left(-1.11 \frac{gO_2}{gN} \right) \cdot \left(-1 \frac{gTOD}{gO_2} \right) + \left(-1 \frac{gN}{gN} \right) \cdot \left(-3.43 \frac{gTOD}{gN} \right) + 1 \frac{gN}{gN} \cdot \left(-4.56 \frac{gTOD}{gN} \right) + v_{2,5} \cdot 1 \frac{gTOD}{gCOD} = 0$$

$$v_{2,5} = 0.02 \frac{gCOD}{gN}$$

The results are summarized in table 1.

Table 1: Stoichiometric and Composition Matrix for Nitritation and Nitratation

Process j	Material i				
	Oxygen $S_{O_2} gO_2$	Ammonium $S_{NH} gN$	Nitrite $S_{NO_2} gN$	Nitrate $S_{NO_3} gN$	Biomass X gCOD
Nitritation	-3.22	-1	+1		+0.21
Nitratation	-1.11	0	-1	+1	+0.02
Units of coefficients	$\left[\frac{gO_2}{gN} \right]$	$\left[\frac{gN}{gN} \right]$	$\left[\frac{gN}{gN} \right]$	$\left[\frac{gN}{gN} \right]$	$\left[\frac{gCOD}{gN} \right]$
Conservatives k					
gTOD	-1 $\left[\frac{gTOD}{gO_2} \right]$	0 $\left[\frac{gTOD}{gN} \right]$	-3.43 $\left[\frac{gTOD}{gN} \right]$	-4.56 $\left[\frac{gTOD}{gN} \right]$	1 $\left[\frac{gTOD}{gCOD} \right]$
gN	0 $\left[\frac{gN}{gO_2} \right]$	1 $\left[\frac{gN}{gN} \right]$	1 $\left[\frac{gN}{gN} \right]$	1 $\left[\frac{gN}{gN} \right]$	0 $\left[\frac{gN}{gCOD} \right]$

4. Biomass concentration in sludge

The incoming Ammonium can leave the plant only in the form of Ammonium, Nitrite or Nitrate. (assuming no Denitrification is taking place). If the effluent concentrations of Nitrite and Nitrate are $1gN/m^3$ and $10gN/m^3$ respectively, there have to be $4gN/m^3$ of Ammonium in the effluent.

According to this $11gN/m^3$ are converted into Nitrite and $10gN/m^3$ of those are then nitrified completely to Nitrate. The amount of biomass produced by Nitritation and Nitratation can be calculated with the help of the stoichiometric coefficients.

$$11 \frac{\text{g}N_{NO2}}{\text{m}^3} \cdot 0.21 \frac{\text{g}COD}{\text{g}N_{NO2}} = 2.31 \frac{\text{g}COD}{\text{m}^3}$$

$$10 \frac{\text{g}N_{NO3}}{\text{m}^3} \cdot 0.02 \frac{\text{g}COD}{\text{g}N_{NO3}} = 0.20 \frac{\text{g}COD}{\text{m}^3}$$

The concentration of biomass in the sludge can then be calculated by a mass balance over the influent and all effluents (clarifier and sludge removal).

$$12000 \frac{\text{m}^3}{\text{d}} \cdot 2.51 \frac{\text{g}COD}{\text{m}^3} / 5 \frac{\text{m}^3}{\text{d}} = 6024 \frac{\text{g}COD}{\text{m}^3}$$

The biomass concentration in the sludge amounts to about 6 kg/m³.

5. Steady State concentrations in effluent

The solution of this question requires mass balances for Ammonium, Nitrite and Nitrate in all four reactors, five counting two reactors for the clarifier. An example is given for Nitrite in the first RCB tank, the others can be found in the BM code. The major difference between them is the reaction rate, that has to be adapted for the different species.

$$\frac{dS_{NO2,1}}{dt} = \frac{Q}{V_{RCB}} \cdot (S_{NO2,in} - S_{NO2,1}) + j_{NH4} \cdot \frac{S_{NH,1}}{K_{NH} + S_{NH,1}} \cdot \frac{A_{RCB}}{V_{RCB}} - j_{NO2} \cdot \frac{S_{NO2,1}}{K_{NO2} + S_{NO2,1}} \cdot \frac{A_{RCB}}{V_{RCB}}$$

METHOD RK4

STARTTIME = 0

STOPTIME=10

DT = 1/24/60

;days

;timestep in min

Q=12000

V=100

Vc=1000/2

;m3/d

;m3

;m3

A=20000

SNHin=15

SNO2in=0

SNO3in=0

Xin=0

;m2

;gN/m3

;gN/m3

;gN/m3

;gCOD/m3

;====KINETICS=====

jNH4=4

jNO2=5

KNH4=2

KNO2=1

;gN/m2/d

;gN/m2/d

;gN/m3

;gN/m3

rNH[1..3]=jNH4*SNH[i]/(KNH4+SNH[i])*A/V

rNO[1..3]=jNO2*SNO2[i]/(KNO2+SNO2[i])*A/V

;===MASS BALANCES FOR AMMONIUM===

init SNH[1..3]=1

d/dt(SNH[1])=Q/V*(SNHin-SNH[1])-rNH[1]

d/dt(SNH[2..3])=Q/V*(SNH[i-1]-SNH[i])-rNH[i]

;first RCB

;second and third RCB

```

init SNHc1=1 ;first CSTR of clarifier
d/dt(SNHc1)=Q/Vc*(SNH[3]-SNHc1)

init SNHc2=1 ;second CSTR of clarifier
d/dt(SNHc2)=Q/Vc*(SNHc1-SNHc2)

;===MASS BALANCES FOR NITRITE===
init SNO2[1..3]=1 ;first RCB
d/dt(SNO2[1])=Q/V*(SNO2in-SNO2[1])+rNH[1]-rNO[1]
d/dt(SNO2[2..3])=Q/V*(SNO2[i-1]-SNO2[i])+rNH[i]-rNO[i] ;second and third RCB

init SNO2c1=1 ;first CSTR of clarifier
d/dt(SNO2c1)=Q/Vc*(SNO2[3]-SNO2c1)

init SNO2c2=1 ;second CSTR of clarifier
d/dt(SNO2c2)=Q/Vc*(SNO2c1-SNO2c2)

;===MASS BALANCES FOR NITRATE===
init SNO3[1..3]=1 ;first RCB
d/dt(SNO3[1])=Q/V*(SNO3in-SNO3[1])+rNO[1]
d/dt(SNO3[2..3])=Q/V*(SNO3[i-1]-SNO3[i])+rNO[i] ;second and third RCB

init SNO3c1=1 ;first CSTR of clarifier
d/dt(SNO3c1)=Q/Vc*(SNO3[3]-SNO3c1)

init SNHc2=1 ;second CSTR of clarifier
d/dt(SNHc2)=Q/Vc*(SNHc1-SNHc2)

```

The code results in an effluent concentration of 1.71g/m³ for Ammonium and 0.75g/m³ for Nitrite.

If we don't include the mass balances for Nitrate in the BM code we can estimate the Nitrate effluent concentration by a simple mass balance as we have done in part 4. This is possible because Nitrogen is only present in these three forms and is not removed via the sludge, so all the Ammonium in the influent has to be split up into the three soluble forms. The Nitrate concentration in the effluent is therefore 12.54g/m³, which is also the result from the program.

6. Estimation of kinetic Parameters at Steady State

The possibility of the estimation of parameters depends on their sensitivity. If a parameter is sensitive it can be estimated more easily and more accurately. On the other hand it can happen, that parameters are correlated. This results in the fact, that, if one parameter is changed, the correlated parameter can change in a way to partly or even completely compensate the change of the first parameter. It is not possible to separate the two correlated parameters in cases like this.

To find out if the parameters can be estimated in the described case, we can calculate the sensitivity functions with BM (→Parameters, Sensitivity) and make a visual comparison between the functions of the different parameters. For this, the code in BM has to be changed. BM only calculates the partial derivative as a sensitivity function, so we need to implement a relative parameter to be able to look at the absolute-relative sensitivity functions. This is done as shown in the code below.

By inserting a new array that includes the inflow concentration, the sensitivity functions can be displayed from the inflow of the first RBC tank to the effluent of the third. (Graph → Choose Variables → X Axis: [i])

```

jNH4=4*jNH4rel           ;gN/m2/d
jNH4rel=1

jNO2=5*jNO2rel          ;gN/m2/d
jNO2rel=1

KNH4=2*KNH4rel         ;gN/m3
KNH4rel=1

KNO2=1*KNO2rel         ;gN/m3
KNO2rel=1

;===VARIABLES FOR OUTPUT=====
NO2[1]=SNO2in
NO2[2]=SNO2[1]
NO2[3]=SNO2[2]
NO2[4]=SNO2[3]

NH4[1]=SNHin
NH4[2]=SNH[1]
NH4[3]=SNH[2]
NH4[4]=SNH[3]

```

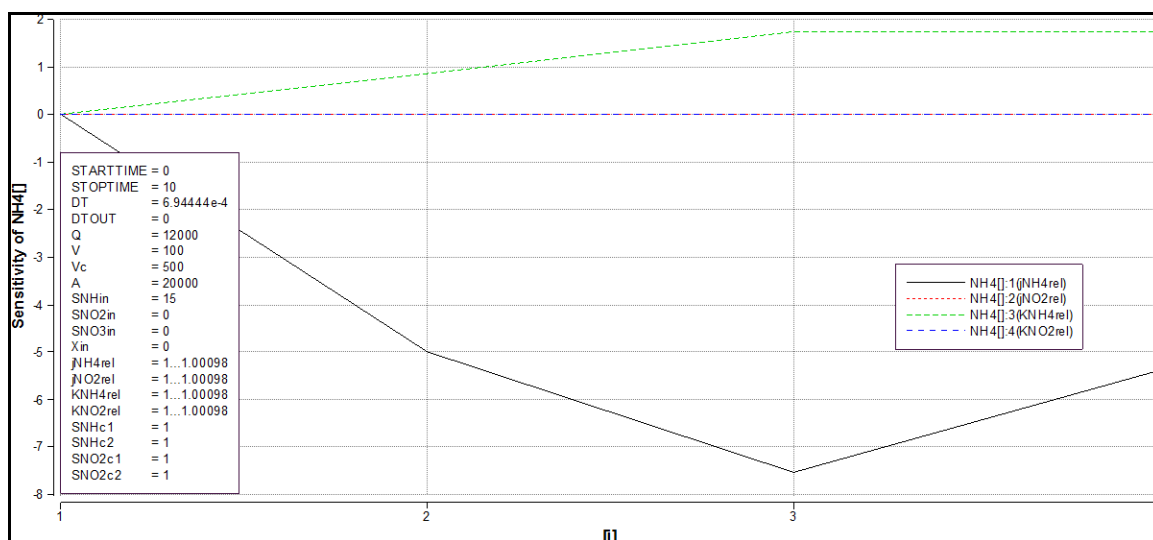


Figure 1: Absolute-relative Sensitivity of Ammonium concentration with respect to the kinetic Parameters

Figure 1 shows the absolute-relative sensitivity functions of the four kinetic parameters with respect to Ammonium. We can see that the Ammonium concentration cannot be used to estimate the parameters KNO2 and jNO2, as the sensitivity functions of those two parameters stays at zero over all three reactors. This makes sense as the Ammonium concentration is not influenced by the Nitrataion reaction, where those two parameters are needed.

The shape of the other two sensitivity functions shows no similarity. It should therefore be possible to estimate the two parameters KNH4 and jNH4 separately from the Ammonium concentrations at the influents and effluents of the four reactors (3 RBC plus 1 SC). With only the results in the influent and in the effluent of the secondary clarifier (or only the effluent of one of

the RBCs) it would not be possible to identify these two parameters (one measurement does not allow to identify two parameters).

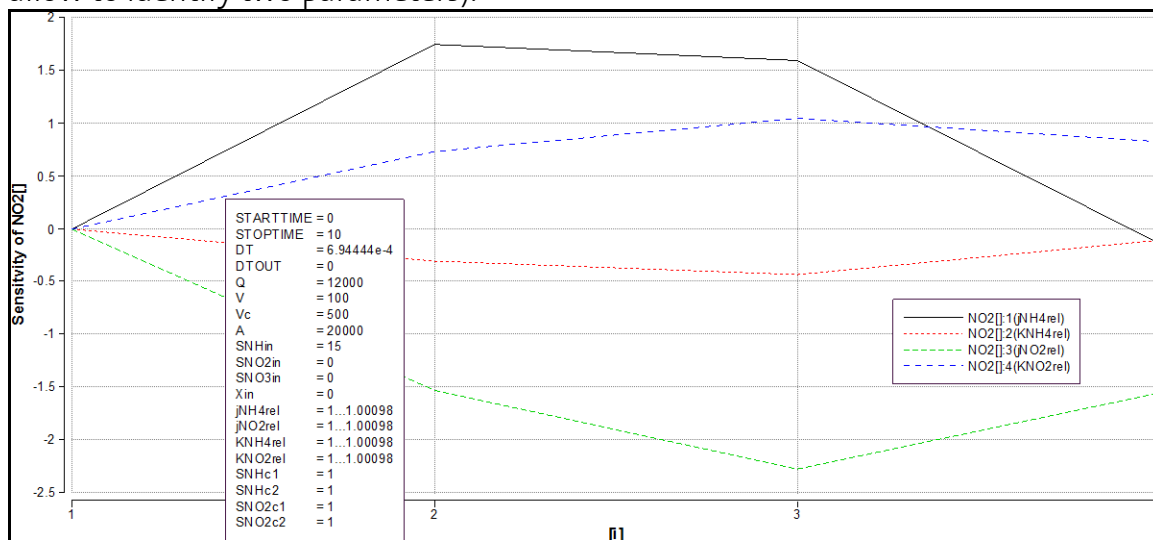


Figure 2: Absolute-relative Sensitivity of Nitrite concentration with respect to the kinetic Parameters

The sensitivity functions in figure 2 show that the parameters j_{NH_4} and K_{NO_2} have unique shapes and it should therefore be possible to estimate them. For K_{NH_4} and j_{NO_2} the picture looks different. The two functions only seem to differ by a factor so it will be difficult to estimate them separately from the Nitrite concentrations. As the Ammonium concentrations can be used to estimate the parameter K_{NH_4} the correlated parameter j_{NO_2} can be estimated subsequently using the estimated value of K_{NH_4} .

According to this analysis all four parameters can be estimated from measured Ammonium and Nitrite concentrations at the in- and effluents of the reactors. However, there might be correlations including more than two parameters that are not appreciated looking at the above graphs.

7. Estimation of kinetic Parameters with Rain event

The rain event is programmed by splitting up the inflow into the normal inflow Q_{norm} and the rain inflow Q_{rain} . The rain inflow is programmed with the pulse. The rest of the code can be left as in part 6, as we again need the absolute-relative sensitivities.

```

Qnorm=12000 ;m3/d
Qrain=12000*SQUAREPULSE(3,0.083) ;m3/d
Q=Qnorm+Qrain ;m3/d

```

The calculated sensitivity functions are shown below in figure 3. Here we assume that we only have data of Ammonium concentrations over time available. This results in only 4 sensitivity functions. It becomes clear that the parameters j_{NO_2} and K_{NO_2} cannot be estimated with this data, as their sensitivity functions are zero over the whole time span. The reason mentioned above also applies here, as those two parameters do not play a role in the calculation of the Ammonium concentration.

The sensitivity functions of the other two parameters vary quite differently, K_{NH} from 1.7 to 1.4 and j_{NH} from -5.3 to -7.2, which means they are not proportional to each other. In addition there

is a small time shift in their response. Thus it appears that these two parameters may very well be estimated from the data.

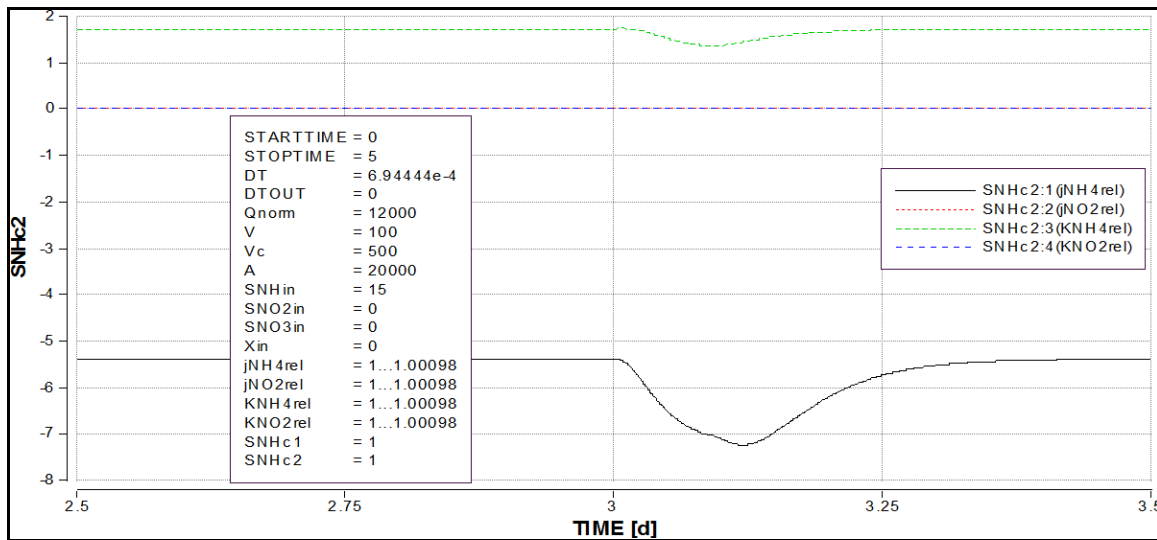


Figure 3: Absolute-relative Sensitivity of the Ammonium concentration with respect to the kinetic Parameters during the rain event

8. Range of Uncertainty of kinetic Parameters

The uncertainty of the kinetic parameters can be implemented in BM via Batch runs (→Parameters, Batch runs, No Parameter). The parameters are made variable and only the mass balances of Ammonium are necessary for the calculation. As the kinetic parameters of the Nitrataion don't influence the Ammonium concentration it is not necessary to implement their uncertainty. The code still shows all the four variables. The code also shows how the maximum value of the effluent can be read out.

```

init jNH4=normal(4,0.6) next jNH4=jNH4 ;gN/m2/d
init jNO2=normal(5,0.75) next jNO2=jNO2 ;gN/m2/d
init KNH4=normal(2,0.3) next KNH4=KNH4 ;gN/m3
init KNO2=normal(1,0.15) next KNO2=KNO2 ;gN/m3

;====FIND MAXIMUM CONCENTRATION====
init SMAX=0
next SMAX=max(SMAX, SNHc2)
  
```

Since the model is non-linear you cannot use a normal distribution to analyse the results. The distribution cannot be described by mean and standard deviation only. Instead you can export the results of the Batch runs in Excel and count the values that exceed 9gN/m^3 . For the ten times conducting 1000 runs the exceedance probability was around 1%. The measurement is therefor compatible but an unlikely result. It is probable that the model does not account for all uncertainties.

Integrated Problem: Analyzing a Fish Pond

1. Procedure

As we cannot enter the property to measure the flow into the pond, we try to find out how much water the owner diverts by a tracer experiment. A certain amount of tracer is put into the brook some meters upstream of the property. The whole amount should be put in at once to approximate a Dirac pulse. Just before the brook enters the property and downstream of the property, just after it leaves, the concentration of tracer has to be monitored. By looking at the time curves of tracer concentration downstream of the property, we can find out how much water is diverted, as the flow out of the pond will change the shape of the concentration curve coming out of the property. If we look at the concentration upstream we can tighten the range of the uncertain parameters. To be able to plan the experiment properly a model should be prepared. It can help to show when the concentration has to be measured and what concentration ranges should be expected in order to use the right equipment and to use the tracer efficiently. This helps to avoid unsuccessful experiments and unnecessary costs.

The brook is a Plug flow reactor with turbulence. We can model the system by looking at the change of concentration after a Dirac pulse with eq. 4.26:

$$C(x,t) = \frac{M}{\sqrt{4 \cdot \pi \cdot D_D \cdot t}} \cdot \exp\left(\frac{-(x - v \cdot t)^2}{4 \cdot D_D \cdot t}\right)$$

where M=mass of tracer, D_D =Dispersion coefficient, x=Length coordinate, v=flow velocity in brook and t=time.

If the tracer is put in 100m upstream of the inflow to the property this is put as $x_0=0$ m. The first interesting concentration is then the one at the inflow to the property at $x_1=100$ m. The brook then flows 500m through the property, so we also need the concentration at $x_2=600$ m. At some point some of the flow is diverted to the pond. This can be modelled with a mass balance over a completely mixed tank reactor:

$$\frac{dCP}{dt} = \frac{QP}{Vol} (C(x_2, t) - CP)$$

where CP=concentration in pond, QP=flow diverted to pond, Vol=volume of pond.

The outflow of the pond can then be mixed with the water remaining in the brook to find out the concentration leaving the property:

$$C_{out} = (CP \cdot QP + C(x_2, t) \cdot (Q - QP)) / Q$$

For the tracer experiment the order of Plug flow reactor and CSTR does not matter. With the tracer we determine the Residence time distribution of the whole system. The RTD is not influenced by the order of the subsystems.

The volume of the pond is very big compared to the flow in the brook. This influences the result of our experiment in two ways. The concentration coming from the pond is negligible compared to the one in the brook, meaning that the water leaving the pond only dilutes the concentration in the brook. The second point is, that the pond has a very high hydraulic retention time, so it will take the tracer a very long time to clear out of the pond again. But as this concentration is very small, it will be easier and less time consuming to analyse the peak in the brook. The hydraulic retention time of the brook is very small.

$$\theta_{pond} = \frac{Vol}{QP} = \frac{2000m^3}{0.3 \cdot 0.01m^3/s} \approx 8days$$

$$\theta_{brook} = \frac{L}{v} = \frac{500m}{0.5m/s} = 100s$$

In BM the experiment can be implemented with the following code. To find out how much water the owner of the fish pond diverts, the measured curve of the tracer concentration in the brook below the property can be used in BM to fit the parameter (QP) indicating the amount of water flowing into the pond. Make sure that you don't start at Starttime=0! The program won't work because zero will result in the denominator of the concentration equations.

```
METHOD RK4

STARTTIME = 1
STOPTIME=60*60           ;seconds
DT = 1

;Parameters
Q=0.01                   ;+-0.001m3/s
Vol=2000                  ;+-200m3
QP=0.4*Q                  ;m3/s Diversion into pond
v=0.5                     ;+-0.05m/s
D=0.05                    ;m2/s, Dispersion

;measurements
M=1000                    ;g

;Upstream
x1=100                     ;m
C1=M/(sqrt(4*pi*D*time))*exp(-(x1-v*time)*(x1-v*time)/(4*D*time))

;Into Pond
x2=600                     ;m
C2=M/(sqrt(4*pi*D*time))*exp(-(x2-v*time)*(x2-v*time)/(4*D*time))

;In the Pond
init CP=0
d/dt(CP)=QP/Vol*(C2-CP)

;After the Pond
Cout=(C2*(Q-QP)+CP*QP)/Q
```

2. Taking samples

To make sure that the peak coming out of the property is captured, we have to have an idea of when this will happen. The model of the experiment can help us to find this out. Figure 1 shows the concentration curves at the different points in the brook and in the pond during the experiment, assuming expected values and a diversion of 30%. The figure shows that the concentration leaving the pond is four magnitudes smaller than the one entering it, so dilution in the pond is very high. The peak of concentration downstream of the property occurs at about 20min after the input of the tracer, so measurements should be taken every minute starting 5min before and ending 5min after this moment to make sure that the peak is captured.

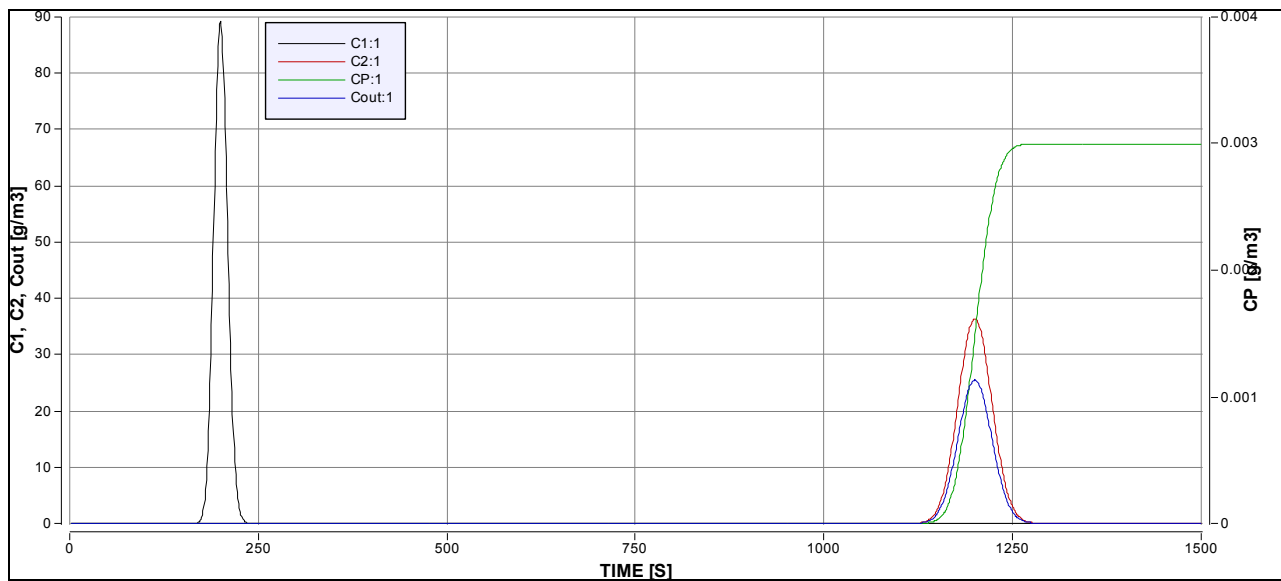


Figure 1: Time course of tracer concentration upstream of the property (C1), at the pond (C2), in the pond (CP) and downstream of the property (Cout)

As the parameters are all quite uncertain their uncertainty should be taken into account. This can be done by implementing them as random variables in BM and conducting Batch runs. We are interested in the magnitude of the concentration peak and the time of its occurrence. Based on the mean and standard deviation of the parameters and Monte Carlo Simulation we get an idea of the expected values and the standard deviation of the predicted behaviour.

The changes in the BM code are shown below.

```

init Q=normal(0.01,0.001) next Q=Q ;m3/s
init Vol=normal(2000,200) next Vol=Vol ;m3
init v=normal(0.5,0.05) next v=v ;m/s

init Coutmax=0 next Coutmax=max(Coutmax,Cout)
init Tmax=0 next Tmax=if Coutmax-Cout<0 then time else Tmax
    
```

5000 Batch runs lead to a mean of the maximum outflow concentration of about 25g/m^3 and a standard deviation of 1.28g/m^3 . The time of the peak averages at 1213s, so very close to the 20min calculated above, and a standard deviation of 125s. The plan mentioned above should be appropriate to capture the concentration wave.

3. Going to court

In order to make sure that we don't accuse the owner without convincing evidence we can conduct the same Batch runs again, now with a diversion of 40%. This can show us if our measurements lie in this range and if we can even distinguish the results of the 30% and 40% diversions.

The mean of the maximum concentration results at 22g/m^3 with a standard deviation of 1.08g/m^3 . The time of the peak is at 1215s, so nearly the same as for the 30% diversion, with a standard deviation of 123s. The concentrations are very close together and considering a confidence interval of 95%, which equals approximately twice the standard deviation, their distributions overlap. Based on this result I wouldn't be confident enough to accuse the owner.

4. Algae Growth

To model the algae growth we have to take into account the feeding of the fish. We assume that most of the Phosphorous from the food is available in the water as the fish only take up a very small part and the rest is excreted again. The feeding is then modelled as a pulse in the Phosphorus concentration of the inflow to the pond. The Phosphorus amount contained in the 5kg fish food equals 250gP. This is distributed over 5min at midday, so the concentration results from dilution in 5min of inflow:

$$SP_{in} = \frac{250\text{gP}}{0.01\text{m}^3 / \text{s} \cdot 0.3 \cdot 60\text{s} / \text{min} \cdot 5 \text{min}} = 278 \frac{\text{gP}}{\text{m}^3}$$

The missing stoichiometric coefficients in Table 16.25 can be calculated using the conservative Phosphorus. This results in -0.02gP/gTSS and 0.02gP/gTSS for the processes of Growth and Respiration respectively.

If we assume that the algae only grow in the pond as their residence time in the brook from the pond to the outflow from the property is very short, we only have to look at the pond for the model and can then mix the concentration of algae coming out of the pond with the water in the brook that is algae-free. So again we have a dilution.

The code below shows how the problem can be implemented in BM. When the model has reached steady state the concentration of algae in the brook oscillates between 12 and 15gTSS/m^3 over one day. Figure 2 shows the time course of algae in the pond and in the brook and the Phosphorus concentration in the pond over two days, where the start of the day is at 6o'clock in the morning. There is clearly a daily pattern of increasing algae concentrations over the day and a decrease over the night. The input of Phosphorus due to the feeding of the fish is also visible. It gives the algae growth a visible push as the concentration of Phosphorus is approaching zero and the growth is getting slower.

METHOD RK4

STARTTIME = 0

STOPTIME=40

;days

DT = 0.0001

QP=0.3*0.01*60*60*24

;m3/d

Vol=2000

;m3

my=2

;1/d

KP=0.05

;gP/m3

IS=if mod(time,1)<0.5 then sin(2*pi*time) else 0

;light intensity

kR=0.2

;1/d

;Food input

SPin=if (mod(time,1))>=0.25 and mod(time,1)<0.2534 then 50/(0.01*0.3*60) else 0

;at midday;50gP/kg

;Algae growth in pond

init X=40

;gTSS/m3

d/dt(X)=-QP/Vol*X+my*SP/(KP+SP)*IS*X-kR*X

init SP=0.1

;gP/m3

d/dt(SP)=QP/Vol*(SPin-SP)-0.02*my*SP/(KP+SP)*IS*X+0.02*kR*X

;Algae in brook

Xb=X*0.3

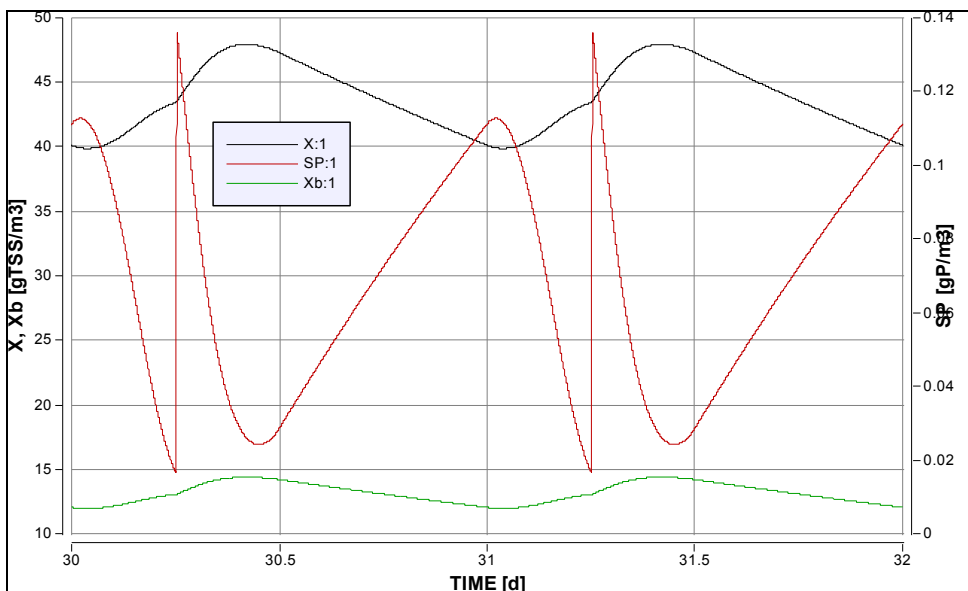


Figure 2: Time course of algae in the pond (X), in the brook (Xb) and Phosphorus concentration in the pond.

5. Addition of Phosphorus

The addition of phosphorus can be modelled by a pulse in Phosphorus concentration at the inflow to the pond. The dispersion caused by the brook on the way from the entrance of the property to the pond can be neglected. More important is the amount of Phosphorus that is

quite substantial. By adding 1kg of Phosphorus the concentration in the pond will increase by about 0.15g/m^3 and will lead to an algae growth of 7.5g/m^3 according to the following equations.

$$\Delta SP = \text{MassP} \cdot \frac{QP}{Q} / V \quad \text{and} \quad \Delta X = \Delta SP / 0.02 \frac{\text{gP}}{\text{gAlgae}}$$

The pulse at the inflow of the pond has to be delayed to make sure that the model is in steady state, which is the case after about 30 days, using the starting values of algae and Phosphorus stated in the BM code. The following code shows a way to implement the problem in BM. Again we have to make sure to start the calculation not at time zero but shortly afterwards. A sensitivity analysis can be done changing the fraction that is diverted into the pond from 0.3 to 0.4

```

METHOD RK4

STARTTIME = 0.0001
STOPTIME=40 ;days
DT = 0.0001

Q=0.01*60*60*24 ;m3/d
fP=0.3 ;fraction of water flowing into pond
QP=Q*fP
Vol=2000 ;m3
my=2 ;1/d
KP=0.05 ;gP/m3
IS=if mod(time,1)<0.5 then sin(2*pi*time) else 0 ;light intensity
kR=0.2 ;1/d

;Pulse of P at pond
M=1000 ;gP
C=pulse(M/Q, 30,1000)

;Food input
SPfood=if (mod(time,1)>=0.25 and mod(time,1)<0.2534) then 50/(0.01*0.3*60) else 0 ;at midday

;P into brook
SPin=SPfood+C

;Algae growth in pond
init X=40 ;gTSS/m3
d/dt(X)=-QP/Vol*X+my*SP/(KP+SP)*IS*X-kR*X

init SP=0.1 ;gP/m3
d/dt(SP)=QP/Vol*(SPin-SP)-0.02*my*SP/(KP+SP)*IS*X+0.02*kR*X

;Algae in brook
Xb=X*0.3

```

Figure 3 shows the time course of the algae concentration in the pond and in the brook and the Phosphorus concentration in the pond for five days before and after the day with the phosphorous pulse. The Phosphorus concentration shows a jump and there is a visible influence on the algae concentrations. The maximum value of algae in the brook after the Phosphorus injection for a diversion of 30% is 16.35gP/m^3 while it is 16.77gP/m^3 for a

diversion of 40% compared to the maxima of 14.38gP/m^3 and 14.30gP/m^3 respectively before the injection. In both cases the maximum occurs on the second day after the injection and then the daily maxima go down again. The change is slightly bigger for the diversion of 40%. But if we think about the high uncertainties of the parameters this does not seem like a significant deviation to find out how much water the owner diverts.

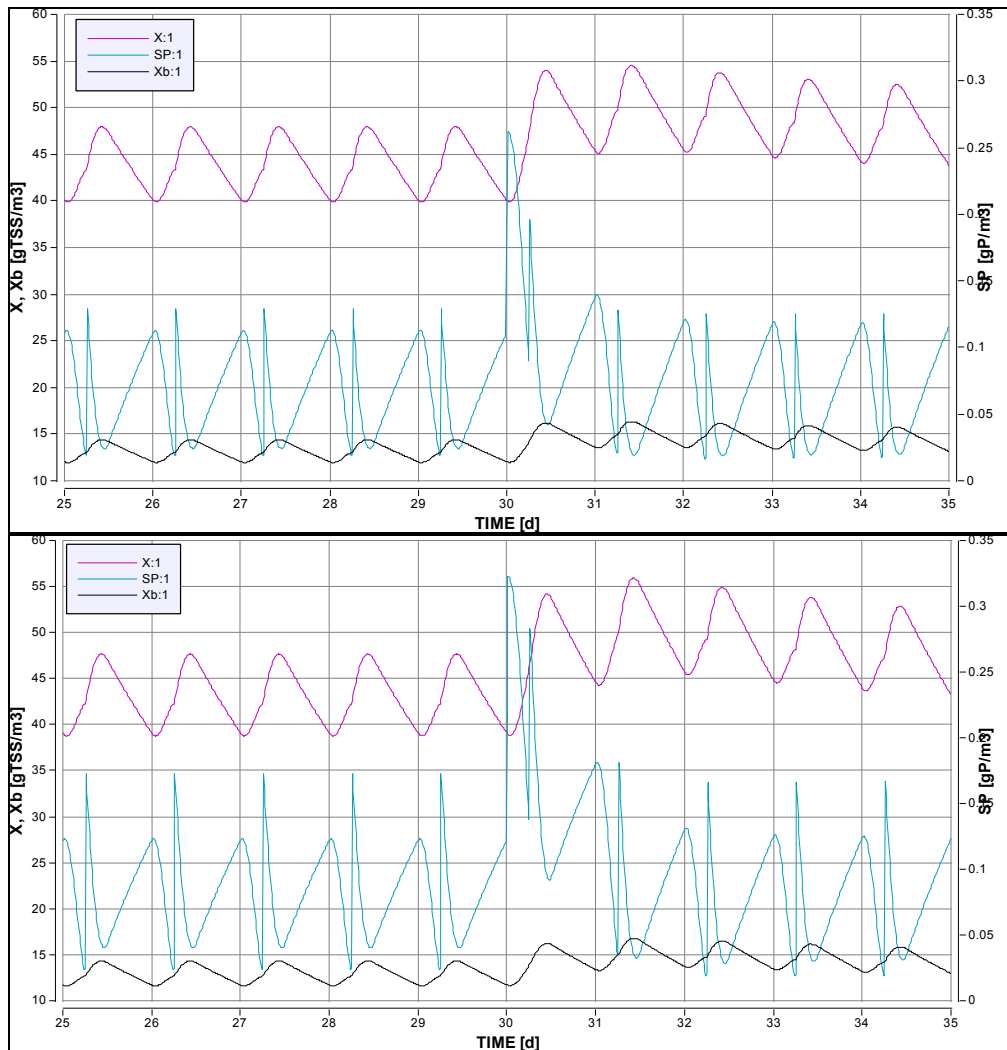


Figure 3: Time course of algae in the pond, in the brook and Phosphorus concentration in the pond for a diversion of 30% on the top and 40% on the bottom.

6. Suggestions for the owner

Probably the easiest and most cost efficient way to reduce the algae growth in the pond would be to decrease the amount of fish food and maintain less fish. Less nutrients would be available in the pond and therefore less algae would grow.

The owner could also divert more water from the brook. This would further dilute the concentrations in the pond and wash out more water into the brook. This would however mean, that the nutrients that are not used in the pond are available in the brook and algae will grow there instead of in the pond.

To reduce growth the input of sunlight could be reduced by planting some trees that cast shadow on the pond. This would cause some costs and again the nutrients, that are not used in the pond will then be available for growth in the brook.

Another possibility is the installation of baffles to simulate a cascade of CSTRs instead of a single pond, this would help to washout the algae (there would not be any algae in a true plug flow reactor).