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Wastewater Treatment Modelling

Wastewater treatment modelling and simulation software

Simulation and prediction of wastewater treatment processes is already required at the stage of designing. These models generally apply dynamic approaches; therefore, the processes and process variables are described in function of time. Unsteady simulations are performed due to the uneven raw wastewater discharge based on the daily, seasonal flow variations and possible industrial sources.

As a result of the unsteady behaviour of the incoming load, the wastewater treatment plant (WWTP) shall not be sized solely for average conditions and the operation should take into account the parameters coming from composite samples rather than using grab samples. Dynamic modelling shall reflect the complexity of wastewater processes, thus the simulation environment is system-based, well-structured and the model elements are similar to an interlocking cog.

The model elements are the following:

- input model: determines the wastewater constituents, fractions and transforms to process modelling variables
- clarifier model: predicts the separation of particulate matter
- biokinetic model: determines the biomass amount required for biological processes and calculates the reactor volumes
- pump model: operation of pumping and calculates energy demand
- sensor model: determines the relation between the measured concentration of the model parameter and the signal of the measurement device
- controller model: gives feedback from the measured value to the operation
- hydraulic and transport model: fluid flow in the reactors and related transport models, including the result of the simplified reactor models originating from multi-dimensional problems
- aeration model: determines the relation between the biological oxygen demand and the air flow introduced to the system through diffusers
- output model: generates composite variables (treated effluent wastewater quality) from the model variables

The connectivity between the model elements is determined by the input and output data. For example, wastewater characterisation provides COD fractions as a result, which is the input data of the biokinetic model. The reactor effluent ammonium concentration determined by the sensor model has effect on air quantity (ammonium control), and thus the aeration and controller models are also affected.

Some model elements are tied closely, e.g. biokinetic and hydraulic model. In this case, one element is idealised in the other sub-model. For example, the complexity of the fluid flow is simplified in biokinetic modelling; the multidimensional behaviour is reduced to its effect on mixing characteristics and assumes well-mixed compartments in the reactor cascade model. Figure 1 represents the model elements and the connectivity among them. This modelling approach was created by the IWA (International Water Association) GMP TG (Good Modelling Practice Task Group).

https://doi.org/10.36250/00881_04

Figure 1

Elements of wastewater modelling (compiled by the author based on [1])

Note: 1: input model; 2: biokinetic model; 3: clarifier model; 4: pump model; 5: sensor model; 6: hydraulic and transport model; 7: controller model; 8: aeration model; 9: output model.

The complex simulation system gives us the opportunity to design, size and operate wastewater treatment processes; predictions, trends, optimisation could be also performed. However, this complexity can be simplified in real life scenarios.

Sizing wastewater treatment processes requires the determination of reactor volumes, the chemicals applied, the aeration demand and the amount of wasted solid. This calculation requires the input model, the biokinetic model, the clarifier model, the aeration model and the output model. User-friendly simulation applications could handle all of the model elements together. There is a huge variety of simulation tools on the market, the following criteria should be considered:

- easy to use, user-friendly platform
- technical support
- upgradability, flexibility
- affordability, value for money

Moreover, a simulation tool is preferred that does not need advanced coding knowledge, provides stable model runs and online support is available. The acquired product should be capable not only for performing general well-known tasks, but it should be upgradable, expandable for specific issues. Price also matters; the value gained by the software (e.g. optimised operation of a WWTP) should cover the costs. It is worth considering, if we have enough experience, to use a free open-source software or a user-friendly simulation environment having technical support for the licensing period. Some selected simulation environment for performing wastewater treatment process modelling:

- Stoat: continuously developing environment with sewerage models, it is advisable for low complexity problems

– WEST: developed by the DHI, flexible environment
– GPS-X: developed by Hydromantis, widespread applications, valuable support; self-developed models (e.g. Mantis model)
– Simba: originally it was spread in German speaking countries, but thanks to the latest improvements it became world-famous
– BioWin: competitor of GPS-X in wastewater industry; complex modelling system in designing and operation of WWTPs; user-friendly environment
– SUMO: new generation tool with high speed simulations

Others simulation tools are AQUASIM, JASS, EFOR, ASIM.

Simulation protocols

It can be seen that a huge variety of models embedded in simulation softwares exist and these have to provide the same results, which is close to the actual conditions. For this purpose and for the comparability of the simulation tools and their results, international protocols were introduced. Some selected simulation tools are the following:

– STOWA protocol: developed by the Dutch Foundation of Applied Water Research, its basis is the Activated Sludge Model Nr. 1 (ASM1)
– Biomath protocol: calibration procedure for the entire ASM model family
– WERF protocol: developed by the Water Environment Research Foundation; it controls the wastewater fractions and introduces multi-level calibration processes
– HSG guideline: general, uses model-independent data

However, the main concept is similar, it is visible that the above-mentioned protocols put emphasis on different processes; the differences are in the details. Consequently, the models applying different protocols are not comparable. The International Water Association (IWA) has an objective to introduce the good modelling practice and standardise wastewater modelling.

Mass balance based (biokinetic) modelling

Biokinetic modelling requires the knowledge of the basic physical, chemical and biological processes and process units. The time dependent processes are based on the required biomass quantity and substrate kinetics.

The conversions of the biological wastewater treatment are the following:

1. growth of the organisms
2. hydrolysis
3. degradation of substrate

Growth of the organisms

Microorganisms in wastewater treatment perform degradation/transition of simple structured molecules for their growth. The molecules used are acetic acid, ethanol, methanol, propionic acid, glucose, ammonium, nitrite, etc. The growth is an enzyme-catalysed reaction and its process

follows the Monod kinetics applying the reproduction kinetics and can be described with the following equation:

$$\mu = \mu_{max} \cdot \frac{S}{K_S + S}$$

where

μ: specific growth rate [t^{-1}]

μ_{max}: maximum specific growth rate [t^{-1}]

S: substrate concentration [mg/l]

K_S: half saturation constant of the substrate, which is the substrate concentration at the half of the maximum specific growth rate [mg/l]

Based on Monod kinetics a yield can be introduced reflecting the amount of biomass (sludge) produced from 1 kg organic matter.

$$\frac{dX}{dt} = Y\frac{dS}{dt}$$

where

X: daily produced biomass amount [kg/d]

S: daily incoming substrate amount [kg/d]

Y: yield [kg/kg]

Based on the above-described equations the kinetic equation for the substrate is the following:

$$\frac{dS}{dt} = \frac{-1}{Y}\mu_{max}\frac{S}{K_S + S}X$$

There could be various kinds of substrates of course; in that case, individual equations shall be written for each substrate.

Hydrolysis

Conversion of the large molecules to smaller size molecules (these can be particulate or dissolved). In this biochemical process, hydrolases – a type of enzyme operating outside the cell (extracellular enzymes) – are responsible for the splitting of large size organic matter (e.g. biopolymer). The resulting smaller molecules could be taken up by the cells and convert to molecules required for the growth and reproduction, and parallel the biomass amount increases. Since hydrolysis kinetics is generally slower compared to biological growth, this process is the "bottleneck" in wastewater treatment.

Decay

Decay of microorganisms is important in the conversions and mass balance of the wastewater treatment processes. By this process, a certain amount of slowly biodegradable substrate is introduced to the system. This can hydrolyse resulting growth causing reduction in dissolved oxygen and/or nitrate concentration.

These were the main conversion processes in wastewater treatment. The removal processes can be divided to organic matter removal, nitrification and denitrification. The model build-up is presented step-by-step in the following. Matrices are used for the structured description, where the processes (rows) and components (columns) are listed.

Step 1: Growth of heterotrophic organism. Anaerobic degradation of dissolved organic matter: the process takes place in the presence of oxygen. It requires dissolved oxygen and heterotrophic biomass. Model components are the following:

– soluble oxygen *(SO_2)*
– soluble biodegradable organic matter *(SS)*
– soluble inert organic matter *(SI)*
– heterotrophic biomass *(XH)*

The components and process matrix can be seen in Table 1.

Table 1
Growth of heterotrophic biomass (compiled by the author)

Component	SO_2	SI	SS	XH
Growth of heterotrophic biomass	$1–1/Y_H$		$–1/Y_H$	+1

The process rate of aerobic heterotrophic growth:

$$\mu_H \cdot \frac{SO_2}{K_{H,O_2} + SO_2} \cdot \frac{SS}{K_{H,SS}} \cdot X_H$$

The model calculates the aerobic heterotrophic growth based on Monod kinetics and takes into account the process rate, oxygen concentration and the biodegradable organic matter. The heterotrophic organism yield is about Y_H= 0.67 g/g, the maximum heterotrophic growth rate is μ_H= 4.1/d. The half saturation coefficient for oxygen is $K_{H,O2}$= 0.2 g O_2/l, the half saturation coefficient for substrate is $K_{H,SS}$= 5.0 g SS/l.

Based on Table 1 and the process rate, the transport equations of the model components are the following:

– soluble oxygen concentration

$$\frac{dSO_2}{dt} = \left(1 - \frac{1}{Y_H}\right) \cdot \mu_H \cdot \frac{SO_2}{K_{H,O_2} + SO_2} \cdot \frac{SS}{K_{H,SS}} \cdot X_H$$

– soluble biodegradable organic matter

$$\frac{dSS}{dt} = \left(\frac{-1}{Y_H}\right) \cdot \mu_H \cdot \frac{SO_2}{K_{H,O_2} + SO_2} \cdot \frac{SS}{K_{H,SS}} \cdot X_H$$

– heterotrophic biomass

$$\frac{dXH}{dt} = (+1) \cdot \mu_H \cdot \frac{SO_2}{K_{H,O_2} + SO_2} \cdot \frac{SS}{K_{H,SS}} \cdot X_H$$

Namely, the component variation over time equals the coefficient coming from the table multiplying with the process rate. In the next step, the model is expanded by lysis, which reflects the decay of microorganisms and conversion to biodegradable matter. In this case, one new process will appear in the matrix, the component number remains the same (Table 2).

Table 2
Growth of heterotrophic biomass (compiled by the author)

Component	SO_2	SI	SS	XH
Growth of heterotrophic biomass	$1–1/Y_H$		$–1/Y_H$	+1
Lysis			+1	–1

It can be seen from the table that the decay of the heterotrophic organisms causes an increase in the biodegradable organic matter. The process rate is proportional to the heterotrophic organisms (=b_H**XH*), where the heterotrophic decay constant is b_H= 0.4 1/d.

Thereby the transport equation for the organic carbon is the following:

$$\frac{dSS}{dt} = \left(\frac{-1}{Y_H}\right) \cdot \mu_H \cdot \frac{SO_2}{K_{H,O_2} + SO_2} \cdot \frac{SS}{K_{H,SS}} \cdot X_H + 1 \cdot b_H * XH$$

Despite the detailed description of the process, the simulations revealed that this equation resulted rapid transition between the biomass and the available substrate. The decomposed cells first form large molecules, then these hydrolyse and split to smaller molecules. In Step 3, the hydrolyses process is introduced to the model system. A new component is needed to be taken into account, which is the slowly biodegradable organic matter. That leads to a change in the lysis process as well; the coefficient of +1 does not belong any more to lysis, but the process of hydrolysis.

Table 3
Decay of organic matter (compiled by the author)

Component	SO_2	SI	SS	XH	XS
Growth of heterotrophic biomass	$1–1/Y_H$		$–1/Y_H$	1	
Lysis			–	–1	+1
Hydrolysis			+1		–1

Hydrolysis process rate:

$$k_H \cdot \frac{XS/XH}{K_X + XS/XH} \cdot \frac{SO_2}{K_{hidr,O_2} + SO_2} \cdot XH$$

where

k_H: kinetic constant of hydrolysis: 1.6 g/g

K_X: half-saturation coefficient for heterotrophic lysis: 0.04 g/g

K_{H,O_2}: half-saturation coefficient for oxygen: 0.1 g O_2/l

The model handles the oxygen consumption appropriately, but underestimates the sludge production. The reason behind this is the fact that the end product of the cell lysis is not entirely biodegradable, particulate inert matter could appear in the system. To develop the model particulate inert fraction of organic matter (*XI*) is introduced. This fraction is about 8% of the biomass (f = 0.08).

Table 4

Aerobic degradation of organic carbon with XI fraction (compiled by the author)

Component	SO_2	SI	SS	XH	XS	XI
Growth of heterotrophic biomass	$1–1/Y_H$		$–1/Y_H$	1		
Lysis				–1	1–f	f
Hydrolysis			1		–1	

Further development of the model could be achieved by the introduction of biological N-removal process, which can happen more conveniently via nitrification and denitrification sub-processes. As a first step, the nitrification shall be built-in the calculation, which results 3 new components in the model. Nitrification is performed by autotrophic organism; therefore, it is necessary to separate the heterotrophic and autotrophic processes. New model components are the autotrophic biomass *(XA),* ammonium-nitrogen *(SNH),* nitrate (nitrite) – nitrogen *(SNO).* New processes are autotrophic growth and the autotrophic lysis. Table 5 can be created by the expansion of Table 4 with 3 components and 2 processes.

Table 5

Organic matter degradation and nitrification (compiled by the author)

Component	SO_2	SI	SS	XH	XS	XI	SNH	SNO	XA
Growth of heterotrophic biomass	$1–1/Y_H$		$–1/Y_H$	+1			$(1–Y_H)/Y_H$*i_N		
Lysis				–1	1–f	f			
Hydrolysis			+1		–1				
Autotrophic growth	$(Y_A–4.57)/Y_A$						$–i_N–1/Y_A$	$1/Y_A$	+1
Autotrophic lysis					1–f	f			–1

autotrophic growth process rate:

$$\mu_A \cdot \frac{SO_2}{K_{A,O_2} + SO_2} \cdot \frac{SNH}{K_{A,SNH}} \cdot X_A$$

autotrophic lysis process rate:

$$b_A \cdot XA$$

In the denitrification process, the heterotrophic growth will be affected and the autotrophic rate remains the same. In anaerobic conditions, the hydrolysis process rate would be slightly different.

Phosphorous removal in wastewater treatment can be a chemical and biological process. Chemical P-removal has three processes: 1. oxidation; 2. precipitate formulation; and 3. re-dissolving. Process parameters can be determined by stoichiometric analysis. Excess biological phosphorous removal is more complex with numerous new components and processes.

Activated sludge models

It was demonstrated that the biokinetic model build-up and extension required various processes and components. It is not necessary to apply the whole set of processes; for a specific case, a subset of processes and components could be enough. The most widespread modelling family is the activated sludge model developed by IWA.

ASM1 – Activated Sludge Model

The model includes 13 components and 8 processes which covers the oxygen consumption, sludge production, carbon and nitrogen mass balance. The task group tried to find equilibrium between the crowd of equations and the completeness of the processes, i.e. reduced the computational cost at simple base cases.

The model components are the following:

1. *SI:* soluble inert
2. *SS:* soluble biodegradable inert
3. *XS:* slowly biodegradable particulate
4. *XI:* non-biodegradable particulate inert
5. *XBH:* heterotrophic biomass
6. *XBA:* autotrophic biomass
7. *XP:* inert particulate products
8. *SO:* soluble oxygen
9. *SNO:* soluble nitrite and nitrate
10. *SNH:* soluble ammonium
11. *SND:* soluble organic nitrogen
12. *XND:* particulate organic nitrogen
13. *SALK:* alkalinity

Model processes:

1. Aerobic growth of heterotrophic biomass
2. Anoxic growth of heterotrophic biomass (denitrification)
3. Aerobic growth of autotrophic biomass (nitrification)
4. Decay of heterotrophic biomass

5. Decay of autotrophic biomass
6. Ammonification
7. Aerobic hydrolysis
8. Anoxic hydrolysis

The ASM1 model does not take into account the effect of pH, it assumes constant stoichiometric and process parameters. For the elimination of this restriction ASM2 was released in 1995, and ASM2d in 1999 as an upgraded version. ASM2 calculates the excess biological P removal and chemical P removal. ASM2 includes 19 components and 19 processes; the ASM2d uses also 19 components, but 21 processes.

Nitrogen forms (ammonia, ammonium, nitrite, nitrite) are extended with dinitrogen. There is no separate equation for organic nitrogen fraction, since it is in the other equation. As for the biological process, there are equations for heterotrophic organisms, nitrifying autotrophic organism and phosphate accumulating organism. This latter one covers the storage of fermentation products, intermittent polyphosphate accumulation, growth and lysis of poly-P bacteria. During the lysis, the stored product could be realised. The kinetic parameters in the model have temperature dependence.

ASM3

This model was issued by the development of the ASM1 model. It has 13 components and 12 processes that cover the following:

- hydrolysis is independent of the electron donor, thus it occurs at the same rate under anoxic and aerobic conditions
- anoxic yield differs from the aerobic yield
- biomass decay is based on endogenous respiration
- includes the heterotrophic COD storage
- different anoxic and aerobic nitrification cell lysis is introduced
- alkalinity is introduced as a limitation parameter

ASM3 basically does not include the P-model, but leaves an opportunity to be extended.

Mantis model

The Mantis model originates from ASM1 except for a few modifications; the kinetic parameters are dependent from temperature, aerobic denitrification is introduced and two additional growth processes are introduced: one for autotrophic organisms and one for the heterotrophic organisms at low or high ammonium concentration, where organisms could uptake nitrate as a nutrient source. The role of the aerobic denitrification is to distinguish and set individually the anoxic and aerobic half-saturation coefficients.

Mantis 2 model

Mantis 2 is a comprehensive model and it comes from ASM2d and the Mantis model. It includes the side stream wastewater processes like the struvite precipitation and anammox technology. It

is capable to integrate the sludge line calculation and ADM (Anaerobic Digestion Model) with carbon, nitrogen and phosphorous mass balance modelling. It introduces 48 state variables and 56 processes. Ions (potassium, calcium, magnesium) appear in state variables and precipitation processes are also appropriately described. The processes are the following:

1. Adsorption of colloidal COD to heterotrophic biomass
2. Aerobic hydrolysis of heterotrophic microorganisms: slowly biodegradable substrate transforms to readily biodegradable COD
3. Anoxic hydrolysis
4. Anaerobic hydrolysis
5. Ammonification: converts soluble organic nitrogen to ammonia nitrogen
6. Growth on fermentable substrate using O_2 as electron acceptor
7. Growth on acetate using O_2 as electron acceptor
8. Growth on propionate using O_2 as electron acceptor
9. Growth on fermentable substrate using NO_3 as electron acceptor
10. Growth on acetate using NO_3 as electron acceptor
11. Growth on propionate using NO_3 as electron acceptor
12. Growth on fermentable substrate using NO_2 as electron acceptor
13. Growth on acetate using NO_2 as electron acceptor
14. Growth on propionate using NO_2 as electron acceptor
15. Decay of heterotrophic microorganism
16. Growth of ammonia oxidiser
17. Growth of nitrite oxidiser
18. Decay of ammonia oxidiser
19. Decay of nitrite oxidiser
20. PHA storage by PAO using acetate
21. PHA storage by PAO using propionate
22. PAO growth on PHA using O_2 as electron acceptor
23. XPP storage on PHA using O_2 as electron acceptor
24. PAO growth on PHA using NO_3 as electron acceptor
25. XPP storage on PHA using NO_3 as electron acceptor
26. PAO growth on PHA using NO_2 as electron acceptor
27. XPP storage on PHA using NO_2 as electron acceptor
28. PAO decay
29. XPP lysis
30. PHA lysis
31. Growth of methylotrophs on methanol using O_2 as electron acceptor
32. Growth of methylotrophs on methanol using NO_3 as electron acceptor
33. Growth of methylotrophs on methanol using NO_2 as electron acceptor
34. Decay of methylotrophs
35. Growth of fermentative bacteria at low H_2 partial pressure
36. Growth of fermentative bacteria at high H_2 partial pressure
37. Decay of fermentative biomass
38. Growth of acetogens on propionate
39. Decay of acetogens
40. Growth of hydrogen trophic methanogens

41. Decay of hydrogen trophic methanogens
42. Growth of acetoclastic methanogens
43. Decay of acetoclastic methanogens
44. Growth of anammox organisms
45. Decay of anammox organisms
46. $CaCO_3$ precipitation
47. $MgNH_4PO_4$*$6H_2O$ (struvite) precipitation
48. $MgHPO_4.3H_2O$ precipitation
49. $Ca_3(PO_4)_2$ precipitation
50. $MgCO_3$ precipitation
51. $AlPO_4$ precipitation
52. $FePO_4$ precipitation
53. CO_2 absorption/desorption
54. N_2 absorption/desorption
55. CH_4 absorption/desorption
56. H_2 absorption/desorption

The activated sludge system can be operated as a continuous flow system (Conventional Activated Sludge), but also as a batch system SBR (Sequenced Batch Reactor). SBR also applies suspended biomass for biological processes, but instead of spatial separation, cycles and time based separation is introduced for each process (feed, mixing with or without aeration, settling and decanting). Cycle times provide the basic sizing parameter and in addition, the simulation should be transient.

SBR can be also equipped with aeration and/or MLSS control. MLSS control provides the stable biomass amount in the reactor, which is 3.5–4.5 mg/l in CAS, whereas it is 5.5–6.0 in SBR. The higher MLSS in SBR is due to the compact sludge structure formed in cascaded reactors. As a user input, cycle times needs to be set. Processes may happen parallel; e.g. biological processes could occur during the feed or settling and decanting could happen simultaneously. For modelling purposes, the following processes are defined:

- mix and fill: wastewater discharges and homogenisation
- aerate and fill: provides aerobic condition
- mix only: provides anoxic condition
- aeration only: post-aeration
- settling: with or without biology
- decanting: treated water removal
- settled sludge removal

Previously, only a part of the activated sludge systems was described, the technologies for large WWTPs (e.g. oxidation ditch) were neglected.

Biofilm models

The ASM and related models were developed for activated sludge system, but these models can be applicable for attached growth (biofilm) processes with some extensions. Processes in the attached growth system are the same compared to processes occurring in flocs of suspended biomass; the difference is only the position of the biomass. In the activated sludge system, the biomass is in suspended form and homogenised within the reactor, whereas in biofilm systems the biomass is

attached to a carrier. The carrier can be moving or stationary. If the carrier is at a certain location (fixed) then the fluid flow is not only responsible for providing the necessary mixing intensity, but the substrate shall be transported to the surface of the biofilm and the end products of metabolism shall be transported out of the system. As a consequence, mass balance modelling shall be coupled with hydrodynamic simulations in biofilm systems.

In the biokinetic modelling environment, the total carrier surface area and maximum biofilm thickness are the user input data. This approach assumes that the carrier is evenly distributed within the system. The calculation of the actual biomass amount is based on the surface area and the actual biofilm thickness in the dynamic simulation. Biofilm could be sliced to a certain amount of layers, where each layer has a different substrate concentration; biological activity also differs between the inner and outer layers. Outer layers close to the bulk flow are supplied by oxygen, thus aerobic condition is present. Contrary to this, the inner layer oxygen supply is deteriorated if the biofilm is thick; therefore, anoxic and anaerobic conditions could appear resulting in simultaneous denitrification and enhanced biological P removal in some cases.

Diffusion is the dominant mass transport through biofilm layers, thus it requires an appropriately high level of shearing and local turbulence. The outer biofilm layer has a high importance; thus, this could communicate the bulk flow. On the surface of the biofilm, a laminar boundary layer may form, which has a hydrodynamic resistance and bottleneck of mass transport. Enhancing mass transport between the bulk and biofilm needs to reduce this boundary layer thickness, which is governed by local turbulence and high velocity gradient. The higher the bulk liquid velocity and the biofilm (carrier) surface roughness, the thinner is the laminar boundary layer. Shearing is developed between two fluid layers with different velocities, resulting swirls (rotation), which could increase the transport process efficiency between the biofilm and bulk flow.

Carrier fill is an important parameter, which presents how much water is replaced by the carrier and also shows the volume of the carrier. Total carrier surface area can be calculated by multiplication of the carrier fill with carrier specific surface area. Specific surface area is calculated by the carrier surface area in 1 m^3 of carrier material. The simplified biofilm model assuming constant biofilm width is summarised in Table 6 for soluble states and Table 7 for particulate states.

It can be seen from the Table 6 and Table 7 that transport processes of the soluble and particulate states are different in the process of attachment and detachment. This process is regulated by the erosion velocity; the ± sign shows that if erosion velocity is higher than the attachment velocity then it is a detachment process, if the erosion velocity is smaller than the attachment velocity, the substrate attaches to the biofilm. Model extension is possible with introducing mass transport between two biofilm layers, which is not detailed here.

Improvement of the model is possible by applying dynamic biofilm width. In this case, the previously described processes are still valid, but with the condition that the amount of biomass is in function with time $[V_{b,f} = V_{b,f}(t)]$. The amount of biomass can be calculated by an additional transport equation and it has effect on the soluble and the particulate states; therefore, the transport equation system also needs to be extended.

Many applications are developed for the attached growth system. One classification is about the position of the carrier and water surface, the other takes into account the fixed or moving behaviour of the carrier. Biofilm systems can be trickling filters, submerged rotating biofilm contactors, biofilters and two types of hybrid systems: MBBR-t (Moving Bed Biofilm Reactor) and IFAS (Integrated Fixed Film Activated Sludge) technologies, which are detailed in the following.

Table 6
Fixed biofilm width – soluble states (compiled by the author)

Bulk mass	in layer of *k*	Process name
$\frac{dS_{b,i}(t)}{dt} =$	$\frac{dS_{k,i}(t)}{dt} =$	
$+(S_{,i} - S_{b,i})\frac{Q}{V_b}$		convection
$\sum_{j=1}^{n_p} R_{i,j}$	$\sum_{j=1}^{n_p} R_{i,j}$	biological process/reaction kinetics
$-\sum_{k=1}^{n_l} +D_i(S_{b,i} - S_{k,i}) \cdot \frac{A_{b,k}}{R_d}\frac{1}{V_b}$	$+D_i(S_{k-1,i} - S_{k,i}) \cdot \frac{A}{R_{bfk}}\frac{1}{V_{bfk}}$ $-D_i(S_{k,i} - S_{k+1,i}) \cdot \frac{A}{R_{bfk}}\frac{1}{V_{bfk}}$ $+D_i(S_{b,i} - S_{k,i}) \cdot \frac{A_{b,k}}{R_d}\frac{1}{V_{bfk}}$	diffusion

Table 7
Fixed biofilm width – particulate states (compiled by the author)

Bulk mass	in layer of *k*	Process name
$\frac{dS_{b,i}(t)}{dt} =$	$\frac{dS_{k,i}(t)}{dt} =$	
$+(S_{,i} - S_{b,i})\frac{Q}{V_b}$		convection
$\sum_{j=1}^{n_p} R_{i,j}$	$\sum_{j=1}^{n_p} R_{i,j}$	biological process/reaction kinetics
$-\sum_{k=1}^{n_l} +D_i(S_{b,i} - S_{k,i}) \cdot \frac{A_{b,k}}{R_d}\frac{1}{V_b}$	$+D_i(S_{k-1,i} - S_{k,i}) \cdot \frac{A}{R_{bfk}}\frac{1}{V_{bfk}}$ $-D_i(S_{k,i} - S_{k+1,i}) \cdot \frac{A}{R_{bfk}}\frac{1}{V_{bfk}}$ $+D_i(S_{b,i} - S_{k,i}) \cdot \frac{A_{b,k}}{R_d}\frac{1}{V_{bfk}}$	diffusion
$-\sum_{k=1}^{n_l} S_{b,i}A_{b,k}v_a\frac{1}{V_b}$	$+S_{b,i}A_{b,k}v_a\frac{1}{V_{bfk}}$	attachment
$\pm\sum_{k=1}^{n_l} S_{k,i}A_{b,k}v_e\frac{1}{V_{bfk}}$	$\pm S_{k,i}A_{b,k}v_e\frac{1}{V_{bfk}}$	detachment

Nomenclature: S: solute concentration (mg/l); *Q:* discharge (m^3/s); *R:* mass flux of reaction rate (mg/l.s); *D:* diffusion coefficient (m^2/s); *A:* surface area (m^2); *V:* volume (m^3); *v:* velocity (m/s)
Indexes: b: bulk; *k:* biofilm layer of k; *i:* component in the transport equation; *j:* process variable (e.g. growth; decay; hydrolysis etc.); *p:* number of processes; *bf:* biofilm; *bfk:* biofilm layer; *l:* number of biofilm layers; *a:* attachment; *e:* erosion, detachment

Trickling Filters (TF)

Modelling of trickling filters requires the following assumptions: the wastewater discharge is continuous and loads the reactor evenly. The model does not take into account fouling and is not capable to determine the hydraulic loss. Distribution of raw wastewater flow is not in the model. The mass transport rate between the biofilm and bulk is different for soluble and particulate states; therefore, the time steps are also different in the numerical model.

Figure 2
Trickling Filter [2]

Since there is an inhomogeneity of variables in biofilm systems, the multidimensional modelling need is high, but the computational capacity of a 2D or 3D model is so elevated that these models are often limited to 1D approach. Model inputs are the reactor depth, carrier surface area and specific surface area. The active biomass amount and substrate in biofilm layers are model variables, thus these provide the model output.

Rotating Biofilm Contactor (RBC)

RBC model assumptions are the following: wastewater discharge is continuous, the even load of the reactor is assumed. The model approach does not take into account the fouling and fluid flow is idealised. The rotation speed and the related biofilm detachment are not built in the model. The model elements are the plates; within each plate, biofilm layers are defined. Each biofilm layer assumes completely mixed hydraulics; between the layers, diffusion is the dominant transport process.

Figure 3
Rotating Biofilm Contactor [3]

Three physical parameters as model inputs are needed: effective water volume, carrier volume and carrier specific surface area. From these parameters, the effective biofilm surface area is calculated. If this surface area is multiplied with biofilm width, the total active biomass amount could be determined.

Aerated biofilter

The simplified aerated biofilter model integrates the 1D biofilm model and permanent aeration model. The model uses horizontal biofilm layers and assumes a plug flow reactor model. Wastewater flows vertically from bottom to top through the biofilm layers and oxygen transport is calculated in each layer separately.

Figure 4
Aerated biofilter [4]

Actually, the process is batched due to backwash requirement, but in modelling the mass flows are continuous and the washed-out particles are taken into account as a point-like sink term. Solid capture expresses the retained particles in the model. There is a possibility to run time-dependent model with the actual phase cycle times, but it is worth starting with a simplified permanent model to get a picture of the processes.

Hybrid biofilm systems

Suspended and attached biomass is simultaneously present in hybrid systems. In modelling, the previously detailed ASM models are combined with the 1D biofilm model. Input parameters are the reactor volume, carrier fill and specific surface area of the carrier.

Figure 5
MBBR carriers [5]

Sub-models in wastewater treatment

Wastewater characterisation

Some fractions of the raw wastewater could be unknown; therefore, the model input cannot be set completely by solely on measurement data. In wastewater characterisation, the fractions are determined applying the measured composite parameters. Depending on the data available, the following wastewater characterisation models can be defined:

- BOD based
- COD based
- COD–TSS based

BOD based fractionation requires BOD_5, TKN and TSS values as input. From these, the readily biodegradable substrate, particulate substrate, inert particulate, free ammonia and ammonium

nitrogen, soluble and particulate nitrogen are determined. BOD_5/BOD_∞ ratio is 0.66 by default, which comes from the stoichiometry. This model assumes that BOD_∞ equals to the total biodegradable COD. Soluble BOD_∞ can be measured by filtered sample and then the particulate fraction can also be calculated. By addition of each COD fraction, the total COD can be determined. It also needs to be noted that due the uncertainty and specialty of BOD measurement this approach is not widely used.

COD based fractionation requires total COD, TKN, TP and COD fraction ratios as input. With the help of COD fraction ratios and total COD, each concentration of the COD fraction can be calculated. COD fractions determine the biomass amount, the organic/inorganic ratio, particulate/soluble states ratio and with the help of these, the TSS can be gained. This model approach has less uncertainty over BOD based models, but it requires additional measurements on fraction ratios (e.g. COD measurement from filtered and homogeneous sample, NUR test for readily biodegradable COD etc.)

The advantage of COD–TSS based model is the simple determination of input parameters. For composite parameters, solely total COD and TSS shall be set and the usage of two following ratios is advisable: VSS–TSS ratio and particulate COD–VSS.

Aeration model

Aerobic biological processes require the presence of soluble oxygen. Open reactors could receive oxygen through diffusion from the air, but in large-scale municipal wastewater treatment systems, this is insufficient for biodegradation, thus an aeration system shall be installed. There are two types of aeration systems: 1. surface aerators; and 2. submerged systems. The latter one has advantage in aeration efficiency; therefore, these are applied widespread. Submerged systems could include diffusers, sparger turbines or jets.

Sizing of aeration devices requires the dynamic description of a two phase air-water system. At the initial stage, the oxygen demand of biomass should be determined, which can separate organic matter removal, nitrification and denitrification processes. Organic matter removal and nitrification consume oxygen, whereas denitrification provides chemically bound oxygen (sink term in oxygen concentration transport equation). If all theoretical demands are summed, field conditions, such as oxygen gas dissolution process to water phase shall be taken into account, which shows us the oxygen to be introduced into the system. The last step is to calculate the air quantity that contains the previously determined oxygen amount and with this number, the aeration device can be selected.

Theoretical oxygen demand can be calculated as follows:

$$OC = (f_c \cdot (OU_c - OU_d) + f_n \cdot OU_n)$$

where

OC: total theoretical oxygen demand [kg/d]

*OU*c: oxygen demand for organic matter removal [kg/d] = specific oxygen demand of organic matter multiplied by the removed BOD_5

*OU*d: oxygen from denitrification [kg/d] = 2.9x removed nitrate-nitrogen

*OU*n: oxygen for nitrification [kg/d] = 4.3x nitrified ammonium-nitrogen

f_c, f_n*:* safety factor, which is in function of SRT, population equivalent and load

The next step is to determine the oxygen amount that needs to be introduced into the system:

$$\mathrm{AOTR} = \mathrm{SOTR} * \beta * (C_s - C)/C_s * 1,024^{T-20} * \alpha * F$$

where

AOTR: actual oxygen transfer rate (theoretical oxygen demand) [kg/d]
SOTR: standard oxygen transfer rate (oxygen needed to be introduced into the system) [kg/d]
β: correction factor of salts, surfactants (saturation oxygen concentration ratio in wastewater and in water) = 0.95 [–]
C_s: saturation oxygen concentration at a given pressure and temperature [g/m^3]
C: dissolved oxygen concentration, which is equivalent with DO [g/m^3]
T: wastewater temperature [°C]
F: fouling factor of the diffuser related to diffuser material and clogging, for clean diffuser 0.9 [–]
α*:* correction factor for oxygen diffusion [–]

The correction factor for oxygen diffusion denotes the oxygen mass transfer ratio from gas phase to liquid phase in wastewater and in clean water. It can be stated that this is a transport between two phases from the oxygen side; therefore, the mass transport equation is the following:

$$\frac{\partial C}{\partial t} = \mathrm{KLa} * (C_s - C) - r_m$$

where

KLa: oxygen diffusion coefficient [1/s]
r_m: oxygen consumed by the microorganisms in unit volume and time [g/(m^{3}s)]

Transport equation includes the oxygen from external source and the biological oxygen uptake. For the determination of the *KLa,* the oxygen uptake shall be neglected; therefore, in the laboratory experiment it is advisable to use clear water. This can be performed at the start-up of a wastewater treatment plant. As a first step, the dissolved oxygen shall be removed from the water filled basin by application of e.g. sodium-sulphite and then the oxygen dissolution curve shall be detected. *KLa* can be determined from the slope of the curve, where the axis (time and concentration) is in a logarithmic scale.

The previously calculated actual oxygen demand shall be modified with the air bubble retention time in the system. *SOTE* (Standard Oxygen Transfer Efficiency) reflects the oxygen dissolution in 1 meter. SOTE depends on the aeration system, generally 5–6% is applied, but latest researches revealed that it could be as high as 8–9%. This value has a dependence on the diffuser density as well.

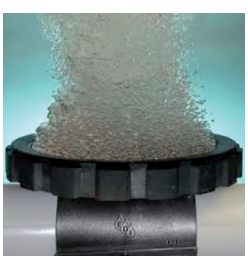

Figure 6
Disc diffuser [6]

In a flow through system, the transport equation shall be extended, the terms are to be multiplied with the reactor volume as follows:

$$V\frac{dC}{dt} = QC_{in} - QC + KLa(C_s - C)V + r_m V$$

where

V: reactor volume [m³]
Q: wastewater discharge [m³/d]
C_{in}*:* oxygen concentration in the influent wastewater [mg/l]

The saturation oxygen concentration depends on the wastewater temperature, the particulate matter, the surfactants, concentration of ions and air pressure. This can be formulated as follows:

$$C_s = \tau \cdot \beta \cdot \omega \cdot C_{s,20°C}$$

where

τ: correction factor for temperature [–]
β: correction factor of particulate matter, surfactants and ions [–] its value is approximately 0.95
ω: pressure correction factor, it can be calculated as follows:

$$\omega = \frac{P_b + p_d - p_v}{P_s + p_d - p_v}$$

where

P_b*:* barometric pressure [Pa]
p_d*:* effective pressure at diffuser depth [Pa] see calculation below
p_v*:* vapour pressure at wastewater temperature [Pa]
P_s*:* standard barometric pressure – 101 325 Pa

The following expression can be used for the determination of barometric pressure:

$$P_b = exp\left[\frac{-gMz}{RT}\right]P_s$$

where

g: gravitational acceleration, 9.81 m/s²
M: molar weight of air, 29 g/mol
R: universal gas constant, 8.314 Nm/mol.K
T: air temperature [K]
z: altitude [m]

The effective pressure at the diffuser depth can be formulated as follows:

$$p_d = (\delta - 1) \cdot (P_s - p_v)$$

where

δ*:* depth correction factor for pressure

fine bubble aeration

$$\delta = 1 + 0.03858 \cdot d$$

coarse bubble aeration

$$\delta = 0.99 + 0.0291 \cdot d$$

where d is the distance between the diffuser position and the water surface

Based on the previous formulae, the *OTR* (Oxygen Transfer Rate) and *SOTR* (Standard Oxygen Transfer Rate) can be calculated:

$$OTR = Kla_T(C_s - C)V$$
$$SOTR = Kla_{20}(C_{20})V$$

Model input for aeration is the volumetric air flow and the achievable DO concentration.

Clarifier model

The clarifier model is a type of the mass transport model, which is based on phase separation and describes the solid phase removal for liquid in gravitational field. The settleable matter can be discrete or group of flocs. The settling of discrete particles can be described by applying Stokes's law if the sedimentation is laminar. The settling velocity depends on the size of particulate matter, the viscosity and the density difference between the solid matter and the fluid. In case of hindered settling, the particles form groups of flocs and the settling velocity is defined for the entire aggregated flocs. This velocity has a function with the solid concentration.

Figure 7
Dorr type clarifier [7]

The homogeneous sample at the initial stage starts to thicken and this makes the phase separation process slower. In clarifiers, the influent flow also interacts with the settling making the process description even more complicated. This complex settling–thickening process can be handled at different levels. In the zero-dimensional models (point models), the incoming and outflowing masses are taken into account and settled solids, which are introduced in the sludge line, can be calculated.

If the settling zone is separated to some layers vertically, we can get the one-dimensional multilayer model. Within this layer, the components are completely stirred. Mass transport may present through the layers due to the concentration difference resulting diffusion, which is not present in real life. This false diffusion (numerical diffusion) may occur if a small amount of layers is applied. Increasing the number of layers, this numerical error can be minimised. Practically 7–11 layers could be enough.

Figure 8 shows the mass flows vertically. The incoming flow *(Q_f)* is separated into two lines: sludge flow *(Q_u)* and treated effluent flow *(Q_e).* In this flow, the settleable solid concentrations are the following: X_f, X_u and X_e. Mass flux between the layers is denoted with *J.*

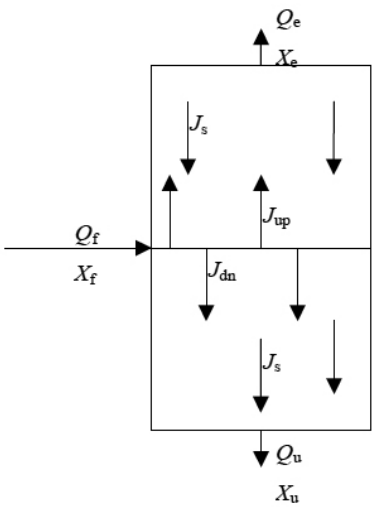

Figure 8
1D vertical multilayer model (compiled by the author)

Continuity (mass balance) for the entire system:

$$Q_f = Q_e + Q_u$$

Component equation can be gained by multiplying the flows with concentrations:

$$Q_f X_f = Q_e X_e + Q_u X_u$$

Mass flux between the layers:

$$J = J_{\text{konv}} + J_s = \text{vX} + v_s X$$

J is the total flux and it is the summation of the convective flux *(J_{conv})* and settling flux *(J)*. (Convective flux can be separated to an upflow and a downflow term. The *v* is the velocity of the flow, v_s is the settling velocity. The general form applying partial differential equation is the following:

$$-\frac{\partial X}{\partial t} = v\frac{\partial X}{\partial y} + \frac{\partial v_s X}{\partial y}$$

For the settling velocity exponential term

$$v_s = k\exp(-\mathrm{nx})$$

or raising to the power of *n*

$$v_s = \mathrm{kX}^n$$

can be applied, where *k* and *n* are settling parameters.

Imre Takács upgraded the previously applied one exponential (Vesilind) model to a two exponential model, incorporating the free and hindered settling. The following formula gives the settling velocity:

$$v_s = v_0\left[\exp(-r_h(x - x_0) - \exp(-r_p(x - x_0)\right]$$

where

v_0: maximum settling velocity in a condition when the settling is free; no hindering effect occurs due to the other particles
r_h: parameter for hindered settling
r_p: settling parameter for low concentrations
x_0: minimum concentration of settleable fraction

Model parameters are determined via laboratory or field measurements. Hamilton extended the above-mentioned scalar transport equation and a pseudo diffusion term was introduced, which is approximately D = 0.54 m²/h.

$$-\frac{\partial X}{\partial t} = v\frac{\partial X}{\partial y} + \frac{\partial v_s X}{\partial y} - D\frac{\partial^2 X}{\partial y^2}$$

With the extension of the 1D settling model, multidimensional hydrodynamic model coupling with mass transport can be formed. It should be noted, however, that the applicability of such models is restricted by the computational cost.

The vertical velocity is now substituted by a two-velocity component field. The velocity values are calculated for each simulation point. With the extension of the turbulent fluid flow, the transport equations are the following:

Continuity

$$\rho\frac{\partial V_x}{\partial x}+\rho\frac{\partial V_y}{\partial y}+\frac{\rho V_y}{y}=0$$

Navier-Stokes (momentum) equation

$$\rho\frac{\partial V_y}{\partial t}+\rho\frac{\partial V_y^2}{\partial x}+\frac{\partial\left(V_xV_y\right)}{\partial x}=-\frac{\partial p}{\partial y}+\frac{1}{y}\frac{\partial}{\partial y}\left(2y\mu_t\frac{\partial V_x}{\partial y}\right)+\frac{\partial}{\partial x}\left[\mu_t\left(\frac{\partial V_x}{\partial y}+\frac{\partial V_y}{\partial x}\right)\right]-2\mu_t\frac{V_y}{y^2}$$

Turbulent kinetic energy

$$\rho\frac{\partial k}{\partial t}+\rho\frac{\partial V_xk}{\partial x}+\frac{\partial\left(V_yk\right)}{\partial y}=\frac{\partial}{\partial x}\left[\left(\mu+\frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x}\right]+\frac{1}{y}\frac{\partial}{\partial y}\left[y\left(\mu+\frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial y}\right]+G_k+G_b-\rho\varepsilon$$

Turbulent dissipation

$$\rho\frac{\partial\varepsilon}{\partial t}+\rho\frac{\partial V_x\varepsilon}{\partial x}+\frac{\partial\left(V_y\varepsilon\right)}{\partial y}$$
$$=\frac{\partial}{\partial x}\left[\left(\mu+\frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial\varepsilon}{\partial x}\right]+\frac{1}{y}\frac{\partial}{\partial y}\left[y\left(\mu+\frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial\varepsilon}{\partial y}\right]+C_1\varepsilon\frac{\varepsilon}{k}\left(G_k-C_3\varepsilon G_b\right)-\rho C_2\varepsilon\frac{\varepsilon^2}{k}$$

Sludge mass transport

$$\rho\frac{\partial C}{\partial t}+\rho\frac{\partial(V_x+V_s)C}{\partial x}+\rho\frac{\partial\left(V_yC\right)}{\partial y}=\frac{\partial}{\partial x}\left(\frac{\mu_t}{\sigma_c}\frac{\partial C}{\partial x}\right)+\frac{1}{y}\frac{\partial}{\partial y}\left(y\frac{\mu_t}{\sigma_c}\frac{\partial C}{\partial y}\right)$$

The settling process is influenced by:

- inflow velocity magnitude
- inflow velocity fluctuation
- geometry of inlet section
- energy dissipation baffle walls
- time for settling
- outlet section

Reactor configurations are not built in (or only in a simplified way) in mass balance models. If the 1D settling model is applied, the settling parameters like SVI (Sludge Volume Index) is fed to the model. SVI or the Mohlmann index (ml/g) is the ratio of settled sludge volume and sludge concentration (SVI = SV30/MLSS). MLSS is the mixed liquor concentration, SVI30 is the volume of settled sludge after 30 minutes of sedimentation. SVI is the general way to describe the sludge settling and thickening behaviour. If SVI is below 100 ml/g the settling is good, if SVI is higher than 150 ml/g the settling is poor.

Controller model

The controller model defines the relation between the process variable and the achievable values (setpoint), e.g. DO = 2.0 mg/l in aerobic reactors. The basis of the control process is the difference between the setpoint and the measured value, which is the error. Disturbance is present in the control process, the setpoint shall be achieved even if there are any disturbances. If the setpoint and measured value are equal, there is no need for the controller to change the status. If the setpoint and measured value are different, the error signal is not zero, the controller shall generate a signal to interfere in the process. The error function is time-dependent [e(t)], and our aim is to minimise the error function in time. As a result of the control process, the system shall be stabilised; in other words, despite the fluctuation in the control parameter due to disturbance it should be relaxed in an equilibrium.

The controller shall consider various attributes of the process. P is the proportional, I is the integral and D is the derivative term. The relation between the control terms is described by the controller term coefficients. The controller terms in the control loop are parallel (see Figure 9).

P: proportional term, the control output is proportional to the control input over time

I: integral of error function, i.e. the residual errors are summed, it may show over prediction in the control output

D: derivative term, shows the changes of error function over time, it increases stability, but it may have a damping effect

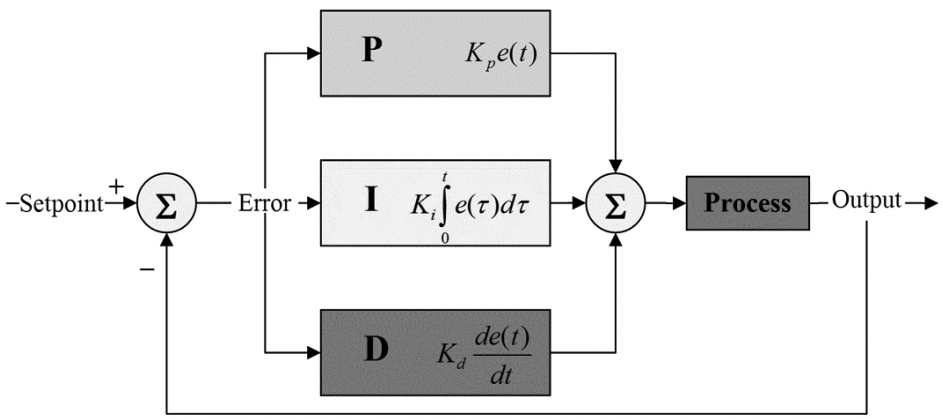

Figure 9
PID control loop [8]

Overall, the control output can be formed as follows:

$$K_p e(t) + K_i \int_0^t e(\tau)d\tau + K_d \frac{de(t)}{dt}$$

Control strategies in wastewater treatment can be classified as follows:

- direct control: the signal reaches the control loop directly
- on/off control: turning on and off could open and close the control loop directly
- cascade control

Cascade control shall be applied if – besides the process variable – another measurable variable exists, which follows the disturbances more rapidly than in the original process variable. This measured variable in the secondary loop filter the disturbance faster than it does in the primary loop.

Cascade control may be applied in the aeration control in biological wastewater treatment that uses the dissolved oxygen concentration as a process variable. DO value is transferred to the control loop and as a control output, the valve in the aeration system is opened and parallel a pressure transmitter transfers signal to the blower to increase its performance (see Figure 10). Higher order of controls also exists: for example, ammonium control calculates the actual oxygen demand based on the measured NH_4-N. Calibration of P, I, D control terms is basically based on measurements, but numerical modelling tools can support the calibration process as well.

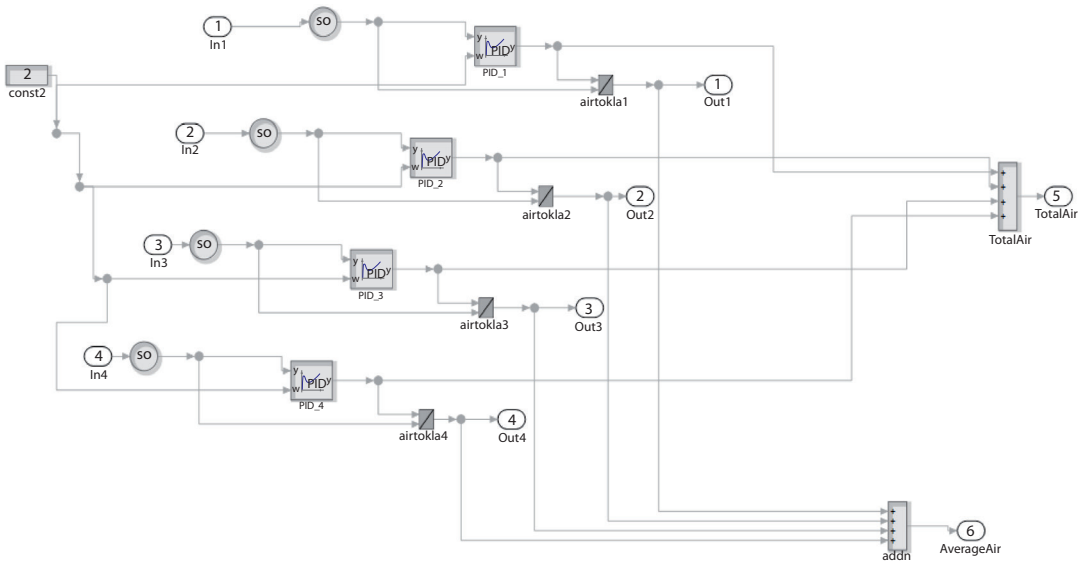

Figure 10
Aeration control loop (compiled by the author)

Reactor models

Ideal and real reactor models

Biological wastewater treatment could take place in concrete basins, or in ditches, natural lakebeds, but whatever the site is, these could be handled as a reactor and reactor models could describe the processes. The classification of reactor models is primarily based on the component distribution within the reactor and the size of the reactors are secondary. If there is no significant concentration difference within the reactor and the concentration varies only with time, the operation can be batch or continuous. One important property of this kind of a reactor is that the effluent concentration equals to the concentration within the reactor.

The reactor mode can be stationary or transient. In stationary reactors, the effluent concentration depends on the influent concentration, whereas in the transient mode not only the influent, but

also the concentration inside the reactor matters. CSTR is a generally applied reactor type that is a Continuous Stirred Tank Reactor, the influent of which is continuous. In PFRs (Plug Flow Reactor), there is a spatial variance in concentration distribution, its mode could be stationary or transient, but as for operation, there is no batch type PFR.

Despite the fact that PFRs have good performance in conversion or biological degradation, they are not widely used in wastewater applications. CSTRs have better mixing properties, thus the influent concentration drops rapidly when it enters the reactor; therefore, the biomass shall not suffer from high load of pollutants and has a less inhibition effect of the process (e.g. heavy metals for nitrification, pH, VFAs).

These reactor types (PFR and CSTR) are idealised regarding the concentration profile. Actually, the completely stirred tank reactor and plug flow reactor without longitudinal dispersion do not exist, the actual condition is somewhere between the two endpoints. It is indispensable to determine the actual reactor model for the estimation of the wastewater treatment performance. Non-ideal reactors can be developed from ideal reactors by introducing one variable (cascade model and dispersion model), two variables (by connecting the ideal reactors) or without using any variables (segregation model, maximum mixedness model). There are two ways to develop a non-ideal reactor model using one variable:

– introducing the dispersion coefficient in PFR; if this coefficient is zero, ideal plug flow can get back, if the dispersion is infinite, CSTR can be formulated
– putting CSTRs in series; ideal CSTR is a one element cascade; if the reactor number tends to infinity, PFR can be gained

It can be seen that two scales can be introduced. One scale depends on the dispersion coefficient, the other uses the number of elements in a CSTR cascade. The two scales are interconnected; therefore, one variable could be useful, which describes the two approaches. For this purpose, the convective and diffusive transport ratio (Peclet number) can be introduced.

$$Pe = \frac{u \cdot L}{D_x} = \text{convective/conductive transport}$$

where

Pe: Peclet number [–]
u: characteristic velocity [m/s], which may be the average velocity within the tank
L: characteristic length [m], which may be a dimension of the tank (regularly the height)
D_x: longitudinal dispersion coefficient [m²/s]

Pe number in wastewater treatment is between 1 and 50, in case of CSTR Pe < 0.5.

The plug flow condition can be present in biofilm systems easily and in this case, the dispersion model is a good choice. Based on operational variables, an optimal Peclet number can be determined, where high biodegradation is expected. The optimal Peclet number changes with the biofilm detachment rate.

It is worth to examine the general transport equation and reformulate it in a dimensionless form:

$$\frac{\partial c}{\partial t} + \underline{u}\nabla c = \mathrm{D}\nabla^2 c + \lambda c$$

where the first term is the concentration changes in time, the second term is the convection (mass transport induced by the flow field). On the right side of the equation are the diffusion term and the first order kinetic term.

The dimensionless form of the transport equation requires the introduction of dimensionless concentration, time and velocity. It should be noted that operator nabla also introduces a division by length scale; * refers to the dimensionless variable.

$$c^* = \frac{c}{S^c}, \qquad t^* = \frac{t}{S_t}, \quad \underline{u}^* = \frac{\underline{u}}{S_{\underline{u}}}, \qquad \nabla( ) = \frac{1}{S_L}\nabla^*$$

By substituting the dimensionless variables:

$$\frac{\partial(c^* \cdot S_c)}{\partial(t^* \cdot S_t)} + \left(\underline{u}^* \cdot S_{\underline{u}} \cdot \frac{1}{S_L}\nabla^*\right) c^* \cdot S_c = D \cdot \frac{1}{S_L^2}\nabla^{*2}(c^* \cdot S_c) + \lambda \cdot c^* \cdot S_c$$

Reordering the variables and constants:

$$\frac{S_c}{S_t} \cdot \frac{\partial c^*}{\partial t^*} + \frac{S_{\underline{u}} S_c}{S_L} \cdot \left(\underline{u}^* \cdot \nabla^*\right) c^* \cdot = D \cdot \frac{S_c}{S_L^2}\nabla^{*2} c^* + \lambda \cdot c^* \cdot S_c$$

By introducing the characteristic time, velocity and length:

$$S_t = \bar{t}, \quad S_{\underline{u}} = \underline{v}, \quad S_L = L$$

dimensionless transport equation can be gained, where the diffusion term includes the reciprocal value of the Peclet number. Since the convective term includes the value of 1, the ratio of convection and diffusion is the Peclet number:

$$1 \cdot \frac{\partial c^*}{\partial t^*} + 1 \cdot \left(\underline{u}^* \cdot \nabla^*\right) c^* \cdot = \frac{D}{\underline{v} \cdot L}\nabla^{*2} c^* + \lambda \cdot \bar{t} \cdot c^*$$

The Pe number is basically influenced by the flow; therefore, it is necessary to know the hydrodynamic conditions of the given reactor and to calculate the convection/diffusion ratio. The determination of this ratio is easily accomplished by a tracer experiment: a tracer is introduced to the liquid stream entering the reactor, and the concentration of the tracer is measured in the effluent (or any other reactor point). The requirement for the tracer is to follow the wastewater flow, not to settle or tend to float, preferably to be conservative, i.e. no chemical reaction. Its concentration in the wastewater should not be comparable to the background concentration (or have information on the background concentration distribution), it should be easily accessible and should not be harmful to the environment. Dosing can be instantaneous or continuous.

If the measurement results of the tracer experiments are plotted against time, a residence time distribution is obtained. It is advisable to normalise the measured tracer concentration with the total amount of tracer introduced into the system to obtain the function of E(t), which reflects

the residence time distribution (RTD: Residence Time Distribution) of the tracer. It is easy to read from the curve that there is a short-circuit and/or dead zone in the system. The hydraulic short-circuit refers to the early appearance of the tracer, and the dead zone is characterised by the trapping of the tracer and is then slowly discharged by turbulent diffusion transport, i.e. the tracer can be measured even after a long time. Figure 11 shows an example of an RTD curve.

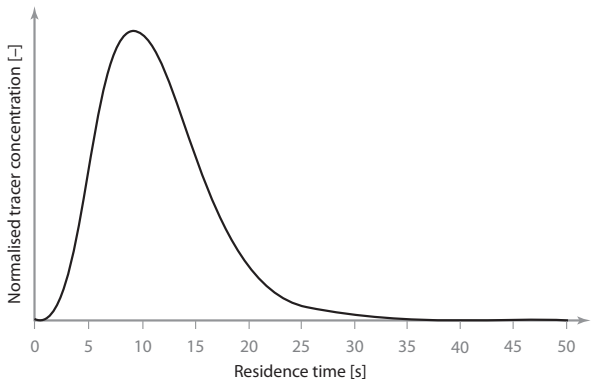

Figure 11
RTD curve (compiled by the author)

The tracer distribution function returned as a result of the RTD analysis – F(t) – can be written as follows by introducing the dimensionless time (Θ), which is defined as the ratio of the elapsed time to the average residence time *(t/t_m)*.

$$F(\theta) = \frac{1}{2}\left[1 - erf\left(\frac{1}{2}\sqrt{Pe}\frac{1-\theta}{\sqrt{\theta}}\right)\right]$$

from this you can obtain the density function, which takes the following form:

$$E(\theta) = \frac{1}{4\sqrt{\pi\,\theta^3/Pe}} exp\left[\frac{-(1-\theta)^2}{4\,\theta/Pe}\right]$$

of which the second-order moment gives the variance of the dimensionless residence time:

$$\sigma_\theta^2 = \frac{\sigma^2}{t_m^2} = \frac{2}{Pe} - 2\left(\frac{1}{Pe}\right)^2 (1 - e^{-Pe})$$

By performing the tracer experiment, we get the RTD curve from which the Peclet number can be determined by statistical tools. If a tank-in-series reactor model is applied, the number of *n* elements can be calculated as follows:

$$n = \frac{1}{\sigma_\theta^2} = \frac{t_m^2}{\sigma^2}$$

from which it follows that, as an approximation, the cascade number is equal to *Pe*/2.

As we have seen, the distribution of the residence time does not determine the biological conversion and thus the effluent concentration, but it can be used to determine a parameter of the real reactor models.

If a tracer study is performed in an existing system, the number of elements of the CSTR cascade is determined, then the result is not necessarily the actual reactor number. As a consequence, the reactor number thus obtained is referred to as the virtual reactor number. Mass balance models in wastewater treatment also shall be fed with this virtual reactor number to provide the actual kinetic process description. In other words, a process engineer who uses the real reactor number in mass balance modelling does not acknowledge the real hydrodynamic conditions, and will idealise the fluid flow, and does not determine the actual reactor size, air and chemical requirements, or sludge yield. It follows that the sizing process must include the virtual reactor elements (these elements can also be referred to as mixing zones). However, experimental tracer tests have several difficulties. It is impossible to perform this test without an existing system. For this case, or for existing systems, numerical analysis could be cost and time effective, if a reliably convergent approximation could be reached at the given hydraulic parameters.

With the help of numerical fluid dynamic simulations (CFD: Computational Fluid Dynamics), the fluid flow of the reactors can be determined by knowing the initial and boundary conditions, the tracer can be introduced into the given velocity field and the RTD analysis can be carried out. Numerical fluid flow simulations solve a partial differential equation system describing fluid movement, including mass balance and momentum equations. In case of turbulent flow, it is necessary to calculate the virtual stress, for which a turbulence model can be used. Among the many turbulence models, the most widespread are the k-ε model assumed isotropic turbulence, or the RSM (Reynolds Stress Model), which applies turbulent stress tensor.

The analytical solution of the partial differential equation system is not possible in case of complex geometries; therefore, numerical method is applied. Finite volume method divides the given reactor volume into finite number of volume elements and solves the equations for each element starting from the boundary and initial conditions. Communication between the cells is possible through the cell interface.

The values of the variables are stored in the centre of the cells, which must be projected onto the boundary of the cell, i.e. interpolated. The result of the calculation depends largely on the numerical scheme used and the resolution that must be independent of the calculation. Because of the number of mesh elements and the magnitude of the numerical capacity, it is mostly an iterative, i.e. step-by-step approach, which must be continued until the solution converges. If a solution converges, the difference between the actual and calculated value is within a range. In this case, the convergence of the calculation can be accepted based on the unchanged iteration residuals or any other variables (e.g. velocity field).

When describing the fluid flow of reactors used in wastewater treatment, the movement of the liquid phase is also influenced by the movement of gas bubbles introduced into the water during aeration. To describe this process, the user could choose among the several multiphase models. The so-called mixture model solves the momentum equations for the primary phase, and a scalar transport equation for the secondary phase, which specifies the volume ratio of the primary phase to the secondary phase for each cell. The primary phase is called the phase that is present in the system at a significantly higher mass. The mixture model may be used if the weight ratio of the secondary phase is less than 10% of the primary phase. If this is not the case, then with the Euler–Euler model, the dynamic equations must also be solved for the secondary phase.

We can apply a multiphase modelling approach even if we only have one component and one phase, but we want to handle and label a part of this flow. This may be necessary for tracer experiments, since the tracer must follow the main flow; it must be the same as all its properties. First, it is worthwhile to run the calculation only for the water phase, and then, at a given time, the tracer is introduced into the system. Then, in the same way as in the physical experiments, the effluent (or any other internal point) concentration is detected and the RTD curve is determined.

However, with this model approach, we may find it difficult to compute, as the tracer will be diluted to a small concentration that can lead to rounding errors. In order to eliminate this, in the model it is advisable to add the tracer from a certain time to the influent, so that the original water phase can no longer be present at the inflow. Influent boundary conditions are determined as follows:

$$0 < t < t0,\ Q(\text{water}) = \text{wastewater discharge},\ Q(\text{tracer}) = 0$$

$$t0 < t,\ Q(\text{water}) = 0,\ Q(\text{tracer}) = \text{wastewater discharge}$$

In this case, the phase ratio of the tracer at the exit point can be increased from 0 to 1 as a function of time. Distribution function of the RTD analysis is given by deriving E(t).

The mass balance and hydrodynamic coupled model can be set up in two ways as discussed above. On the one hand, in the hydrodynamic simulation environment, the range of equations to be solved can be extended with transport models describing the flow. Furthermore, in the mass balance simulation environment, the reactor model can be developed. The method outlined in this chapter is the latter one, the model development involves examining the circumstances that may affect the reactor model. The basin geometry, the discharge, the mixing energy from an external source can influence the current flow field, in which the role of recirculation, aeration and cascading are examined in detail.

The effect of recirculation on the reactor model

There are several types of recirculation streams in wastewater treatment technologies that vary in size and role. The mandatory part of the activated sludge technology is the aerated basin followed by phase separation, where the settled biomass is recycled back to the former basin, resulting in an increase in the sludge retention time (SRT). The primary role of sludge recycling is to maintain the 3–6 g/l biomass concentration in the aeration basin.

The MLE (Modified Ludzack-Ettinger) reactor arrangement uses a pre-denitrification zone in which the anoxic reactor is followed by aerobic (oxic) zone. Nitrification takes place in the aerobic reactor, the final product of nitrate is returned to the anoxic zone by means of recirculation. Thus, nitrate, as an electron acceptor, enters into a zone where the readily biodegradable organic matter, which is essential for heterotrophic microorganisms, is available.

Nitrate recirculation or in other words, the internal recirculation, is generally 1.5–2.5 times the raw wastewater discharge, but it can even reach 4–5 times higher flow in some cases. The actual recirculated water flow is determined empirically. Based on empirical design considerations, it is not advisable to further increase the internal recirculation rate if the NO_3-N concentration is higher than 2 mg/l at the end of the anoxic reactor zone. Conversely, if the NO_3-N concentration is

too low, then the given anoxic space will still be able to further denitrify, so it is worth increasing the internal recirculation.

More complex reactor arrangements can also be developed if we want to combine the biological nitrogen removal with biological excess phosphorus removal. Such a method is, for example, the UCT (University of Capetown) process, where the previously described MLE system is expanded with anaerobic volume used as the first reactor. The reactor sequence is then anaerobic, anoxic, aerobic. Recirculation and their roles:

– sludge recycling from secondary clarifier to anoxic volume – return of biomass
– nitrate recirculation from aerobic to anoxic – returning nitrate to denitrifying microorganisms
– recirculation from anoxic to anaerobic zone – return of biomass

Separation of biomass is important as sludge recirculation cannot directly deliver nitrate to the anaerobic compartment, because there is chemically bounded nitrogen in it. The UCT process assumes perfectly mixed reactors, which means that the nitrate concentration entering the anoxic zone suddenly dilutes, and taking into account the ability of the denitrifier conversion capacity, the effluent nitrate concentration shall be close to zero. If it does not work appropriately, it would inhibit the excess biological phosphorus removal.

It has been mentioned previously that in order to achieve better conversion or degradation, the plug flow reactor should be approached. If the given anoxic volume is divided into two parts, the recirculation from the second reactor with a gradual nitrate concentration profile will probably contain a smaller amount of nitrate-nitrogen. From this idea, the modified UCT procedure has been developed (Figure 12).

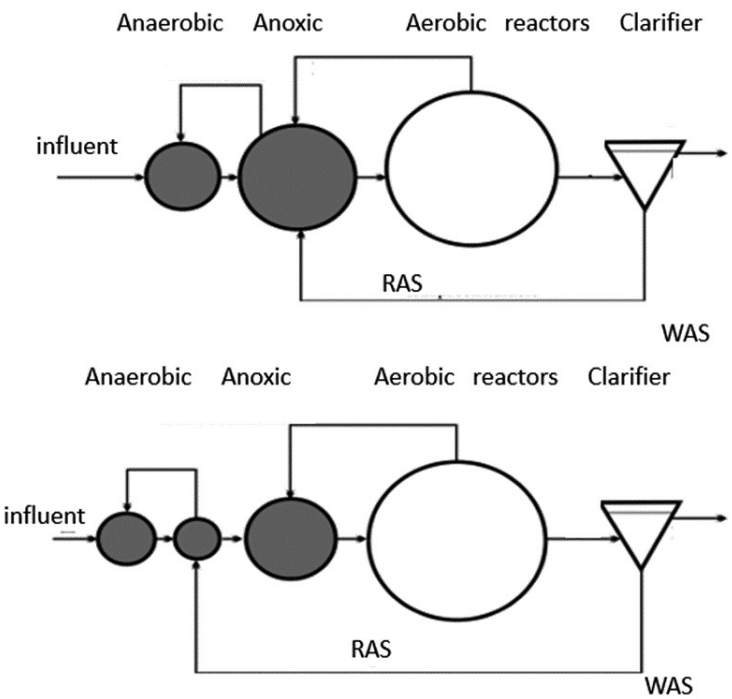

Figure 12
UCT and modified UCT process (compiled by the author)

If the concentration profile of the tank-in-series cascaded reactor should be described, then the concentration inside the tank and effluent concentrations can be calculated by the following formula:

$$C_n = \frac{C_0}{[1 + (k/n \cdot \tau)]^n}$$

where

C_n: concentration in the n -th reactor [g/m^3]
C_0: influent concentration [g/m^3]
k: kinetic constant [1/s]
n: number of reactors [–]
τ: residence time (V/Q) [s]

The formula of residence time has to be upgraded by the increased water flow due to recirculation(s):

$$\tau = \frac{\tau_0}{1 + R}$$

where

R: recirculation ratio [–]

The recirculation ratio expresses how many times higher the flow due to nitrate and sludge recirculation compared to the raw influent wastewater flows. With the introduction of recirculation, the fluid exits faster from the basin since the velocities increase significantly in the tank. The concentration profile also changes, the shorter residence time calculated by the above formula results in a higher effluent concentration. However, these assumptions significantly simplify the kinetics of the biological processes.

GPS-X 6.5 is a simulation environment developed by the Hydromantis mass balance modelling and is applied to determine how the reactor model is affected by recirculation. For demonstration purposes, an existing plant in Hungary with MLE process was investigated.

The effect of aeration on the reactor model

Biological wastewater treatment is mostly carried out by aerobic microorganisms, whose living conditions require the presence of dissolved oxygen. Oxygen can naturally be dissolved in the water following the Henry-theorem, but the biomass used in intensive technologies consumes oxygen much faster than the oxygen dissolution. Furthermore, the dissolved oxygen concentration must be maintained at least at 1.8 to 2.0 mg/l to diffuse the oxygen into the activated sludge flocs (or in case of biofilm systems diffuse to the inner biofilm layers). For this purpose, oxygen is supplied to the water phase by using external energy, which ultimately results in better mixing by the bubbles introduced. Since the basis of the reactor models is hydrodynamics and the aeration rearranges the energetic conditions of the fluid, its effect can be significant. In the following, the aeration requirement is discussed from the design point of view, then the flow generated by the air is examined, and finally the effect of this altered flow field on the reactor model is analysed.

The aeration systems used in wastewater treatment can be divided into two tiers, surface (vertical and horizontal) and subsurface aeration. Aeration systems are expected to have the most efficient oxygen transport, which is measured by the energy delivered projected to one kg of oxygen introduced to the system. Based on the result, the surface aerators are not widely used in everyday practice any more, subsurface aeration (diffusers) are more common. The diffusers are located close to the bottom of the basin, and these can be plate, tube or disc diffusers. Generally, better oxygen diffusion efficiency is achievable in deep basins, but for construction and operational considerations, there is a limit for a depth of about 5 m.

Aeration has effect on the flow field in the reactor, generating vertical flow in a basically horizontal through flow basin and it helps in mixing. Generally, the diffuser distribution is uneven in the basin, the upward and downward circulating zones are separated. The performance of a given reactor depends to a large extent on the fluid flow that depends on the diffuser distribution.

However, it follows that the design basically determines what the plant will probably perform later, during the operation. Operation could have effect via process parameters, but the hydrodynamic conditions rely merely on the pre-defined design parameters. From this point of view, it is crucial to know the fluid flow in detail in the design phase, but this is often neglected in practice. However, the system is complex at such a level that each individual basin should be subjected to undergo hydrodynamic analysis separately.

Physical testing is not possible before the construction of the basin; therefore, CFD analysis should be performed, even if there are guidelines for diffuser distribution pattern to use. The hydrodynamic calculations should incorporate RTD analysis, since the aeration has also effect on the RTD curve. Aeration primarily increases turbulent diffusion, but convective transport also cannot be neglected. From the point of view of reactor models, all these statements mean that, for example, if the reactor is a plug flow type with high Pe number, the Peclet number starts to decrease as the diffusion increases.

The above-described process primarily analysed the macro-effect of the aeration, which can help in particular with the biofilm systems applying fixed film. Since the biofilm is attached to a carrier, the flow plays a role in delivering the substrate to the biofilm surface and removes the end products from the biofilm surface. Organic load on the biofilm attached to a carrier differs at each location within the basin; therefore, various microbial compositions of biofilm can be observed at the beginning and end of the reactor: first we encounter heterotrophic organisms, while samples taken from the end of the basin show the autotrophic dominance responsible for nitrification. In fixed film systems, the placement of mechanical mixers is difficult; therefore, aeration is primarily responsible for mixing. It is sometimes necessary to use aeration in the anoxic reactor, preferably with a coarse bubble size and with intermittent operation. In the latter case, efficient mixing is achieved at conditions where the oxygen dissolution is the lowest.

From the point of view of reactor models, the macro description is sufficient, but it is worth examining the micro-level analysis of the liquid-air multiphase flow. The model should describe the evolution of the initial bubble diameter (adhesion to other bubbles), the break-up of the bubble, and the momentum transfer between the gas and fluid. To solve the complex problem, an anisotropic turbulence model of multiphase flows, large eddy simulation, or direct numerical simulation can be used.

Bubble dynamics is primarily determined by rising velocity, but it is also influenced by the horizontal flow of wastewater. As the bubbles are rising, the drag force has a downward position; the magnitude of the force depends on the shape and velocity of the bubbles. Behind the bubble,

there may be a dead zone (with a function of the Reynolds number) and the swirls from the bubble surface can deflect the vertical motion. Therefore, transient phenomena can be observed with constant background flow and constant airflow rate, as the "bubble plume" develops. The plume is expanding towards the water surface. When placing the diffusers, attention should be paid to the development of the quasi-free flow, i.e. the development of the air-driven flow giving the appropriate space for the flow zone. If there is no free flow, so-called airlift reactors can also be created as alternatives to pneumatic loop reactors. The zones with different densities are used to create upward and downward zones. The microbubbles are injected into the reactor with a 10–100 Reynolds number, the liquid oscillation helps to prevent the bubbles from becoming larger, thus providing a longer residence time and a larger contact area, resulting in the circulation zone being multiple times the reactor depth.

Sludge reduction by cascading the reactors

So far, we have seen the effect of reactor volumes (reactor geometry) and aeration on the fluid flow, which are two output design parameters out of three. However, the third design parameter, the amount of sludge production, is a consequence of reactor designs, i.e. it does not affect the reactor model, but contrary, it is a result. Further on, the effect of different reactor models on sludge yield is analysed.

The sludge yield shows the amount of solids generated in the wastewater treatment plant in one day. This amount should be wasted every day to keep the biomass in balance during biological cleaning. However, it follows that × kg/d dry matter (TS: Total Solid) appears on the sludge line to be treated. In addition to the total dry solid, sludge contains a significant amount of sludge, many of which can be removed mechanically or by chemical dosing during thickening and dewatering. However, these methods focus on reducing the sludge volume and not on reducing the solids content. Sludge is wasted from primary clarifiers, in biological treatment (wasted activated sludge or detached biofilm) or from chemical P precipitation.

Specific sludge yield can be introduced which compares the amount of sludge generated to an input quantity, such as BOD_5 or COD. There is no consensus of what rate should be used; therefore, it is possible to use the TSS/COD, TSS/BOD_5, VSS/BOD_5 ratios, each of course having different values. This specific quantity depends on the sludge age (SRT) significantly; the higher the SRT, the lower the sludge yield. However, the total oxidation of sludge requires not only a large reactor size, but also consumes more oxygen.

Reducing sludge yields can be done at aerobic or anaerobic environment, but where it is possible, anaerobic solutions are preferred, since energy recovery can be achieved. Anaerobic treatment, which is often connected with pre-treatment, is only possible at high capacity plants. In smaller municipalities, however, the reduction of sludge yield is a fundamental interest. One type of solution is based on accelerating the reuse of cellular material after cell death, i.e. cell lysis is promoted by external intervention. The released substances can form new cells that are involved in biological processes. This type of reproduction is also called cryptic growth. Cell lysis can be done mechanically by using ultrasonic or hydrodynamic cavitation or other shearing technologies or with chemicals (chlorination, ozone) or heat treatment.

Another option to reduce sludge yield is to maximise the energy required for maintenance processes. Part of the energy of the microorganisms is focused on maintenance, which includes

the renewal, maintenance of the cellular material, the transport of the nutrient through the cell membrane, and the other part of the energy creates new cellular material. The aim is not to make the latter significant, that is to say, should not have high microorganism growth and high sludge mass. Maximising maintenance energy in municipal wastewater treatment can be achieved through low nutrient supply, chemicals, or changes in the oxic/anoxic environment.

One such method is the OSA procedure, which refers to the alteration of the oxic-sedimentation-anaerobic processes. The settled sludge is "starved" in the anaerobic basin on the side of the sludge recirculation, and when returned to oxic conditions, the substrate obtained is primarily used for rebuilding itself and not for reproduction. However, if the anaerobic basin is designed for the entire recirculated sludge stream, then an unnecessarily large volume is obtained. Experiments have shown that it is sufficient to separate some of the recycled sludge and lead it to a separate reactor where aeration is controlled, with very low dissolved oxygen concentration. After the "shock", the sludge is directed back to the aeration pool.

Primarily due to the high sludge age and the localisation of biomass in biofilm systems, it may happen that higher order organisms live with predation by lower order organisms, which also results in sludge reduction. However, it also appears that the plug flow reactor or cascaded reactor favours the reduction of the sludge yield of the waterline, which can be attributed to protozoa and flagellant organisms as higher order organisms. For their development the following conditions should be fulfilled, DO = 1–3 mg/l, TKN < 30 mg/l, BOD_5 < 530 mg/l, which occurs at the end of the biological basin. The development of the food chain is also advantageous to us, because the nutrient conversion of the superior bodies is weaker and the energy loss is higher. In addition, metazoids reduce the turbidity of water by consuming freely floating bacteria. According to literature, sludge production can be reduced by up to 20–40%, but two-stage cleaning is recommended in an activated sludge system.

Mass balance modelling for individual wastewater treatment unit

Raw influent characterisation, model setup

The GPS-X 6.5 simulation system was used to perform analysis in a certain small wastewater treatment unit. The purpose of the modelling was to determine the actual capacity. The treated wastewater quality can be calculated by setting the raw wastewater quality and the small equipment parameters in the mass balance model.

The test system was a small treatment unit of the Polydox 50 type discussed in detail in *Annex: Examples for Individual Wastewater Treatment Units,* the capacity of which was provided by the manufacturer in 50 population equivalents and 6.0 m^3/d of wastewater. The unit has a volume of 8.4 m^3, from this 70% is aerated and the rest is for clarification and sludge thickening.

In terms of inlet, two types of wastewater were tested according to the water consumption and the associated daily wastewater discharge. On this basis, we distinguish Central European average wastewater and concentrated wastewater. In terms of organic matter, COD varies between 750–1200 mg/l, BOD_5 between 300–650 mg/l, TKN and TP are relatively high compared to other countries.

Table 8
Raw influent characteristic (compiled by the author)

mg/l	average wastewater	concentrated wastewater
COD	750	1,200
BOD_5	310	650
TSS	400	800
TKN	80	100
TP	12	18

In the absence of field data, the following COD fractions were determined in the COD–TSS-based fractionation in the average influent:

- soluble inert COD: 16 mg/l
- readily biodegradable COD: 62 mg/l
- particulate inert COD: 270 mg/l
- slowly biodegradable COD: 402 mg/l
- substrate fraction of the particulate COD: 0.6 mg/l
- organic content of the total suspended solids: 0.8 mg/l

In case of concentrated wastewater, the COD fractions were as follows:

- soluble inert COD: 24 mg/l
- readily biodegradable COD: 96 mg/l
- particulate inert COD: 194 mg/l
- slowly biodegradable COD: 886 mg/l
- substrate fraction of the particulate COD: 0.82 mg/l
- organic content of the total suspended solids: 0.75 mg/l

Simulations performed and results

The model layout is shown in Figure 13, where it can be seen that in addition to the incoming raw wastewater, other wastewater sources can be specified (septage: municipal liquid waste). The wastewater is transported to a buffer tank with a function of equalisation. Thereafter, the biological processes occur, which is aerated. In the model, it is also possible to add external carbon source and/or chemical. The aerated basin is followed by a clarifier where most of the biomass is retained and returned to the system after thickening. The thickening/dewatering combined unit has been set to about 5% solid capture. Treated wastewater flows to a storage tank at the end of the process. The model does not take this further into account.

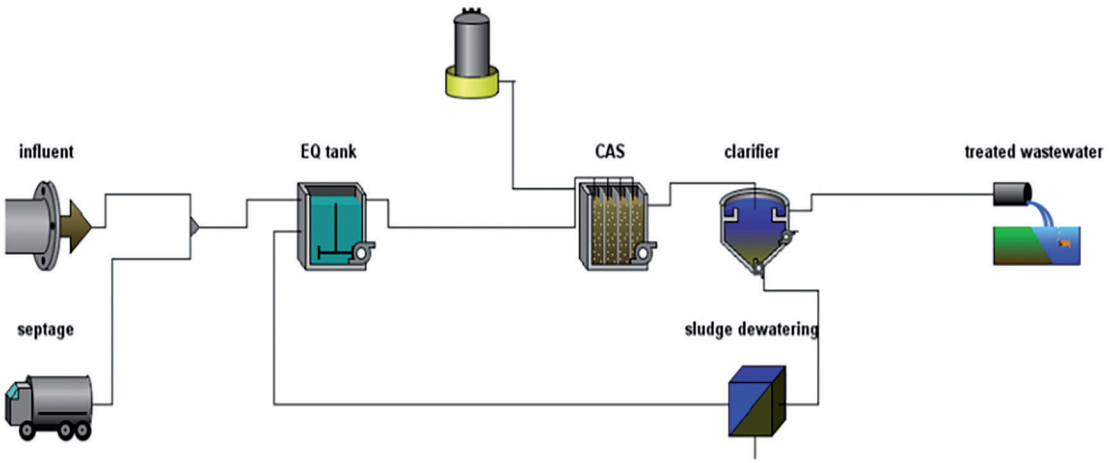

Figure 13
Conventional activated sludge GPS-X 6.5 model layout (compiled by the author)

Steady-state model runs were performed. In the first step, the nominal load of 6.0 m^3/d was taken into account. The dissolved oxygen concentration was 2.0 mg/l in the aerated basin. The sludge production was 1.35 kgTS/d and the dry solid content was 0.78%. The amount of thickened and dewatered sludge is 6.4 l/d. Quality of effluent:

- COD: 50 mg/l
- TSS: 24 mg/l
- NH_4-N: 25 mg/l
- TN: 27 mg/l

This shows partial nitrification; nutrient removal does not happen if the nominal capacity is taken into account. In the next step, nitrification efficiency was determined in function of the amount of influent flow. This could be done in several steps, iteratively, with the trial and error method. As a result of the runs, the wastewater systems could treat approximately 50% of the incoming flow based on the average Central European wastewater quality. If concentrated wastewater quality was considered, it is an additional 20% capacity reduction. In this latter case, it is recommended to increase the operating parameters, i.e. DO = 2.0 mg/l to increase to DO = 3.0 mg/l to avoid capacity loss.

Simulations revealed that despite the steady-state incoming load, there are variations in the effluent in the first few days. The reason for this is that initially there was no biomass in the system and it had to be built. While the biomass was built up, biodegradation was limited. For this, as can be seen from the following series of figures, it took about 10–12 days. Figure 14 shows the TSS and its organic content, the VSS. About 60 mg/l of suspended solids remained in the biologically treated wastewater (without sedimentation). After sedimentation, it decreased further to 5–10 mg/l.

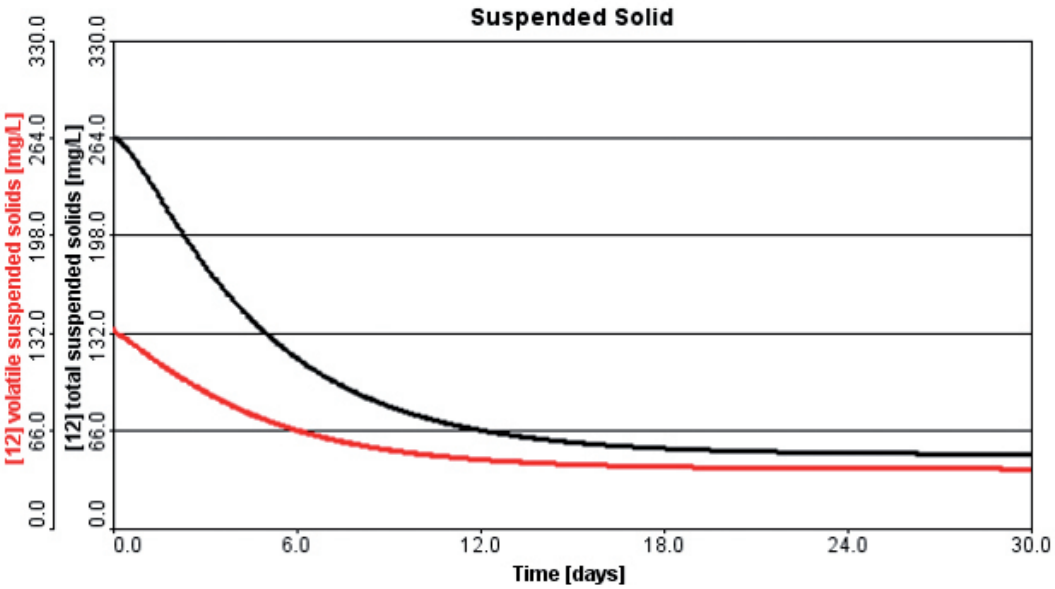

Figure 14
Treated effluent TSS and VSS (compiled by the author)

With respect to organic matter, the effluent COD concentration was 68 mg/l, which is more than 90% treatment efficiency. BOD_5 decreased to 20 mg/l.

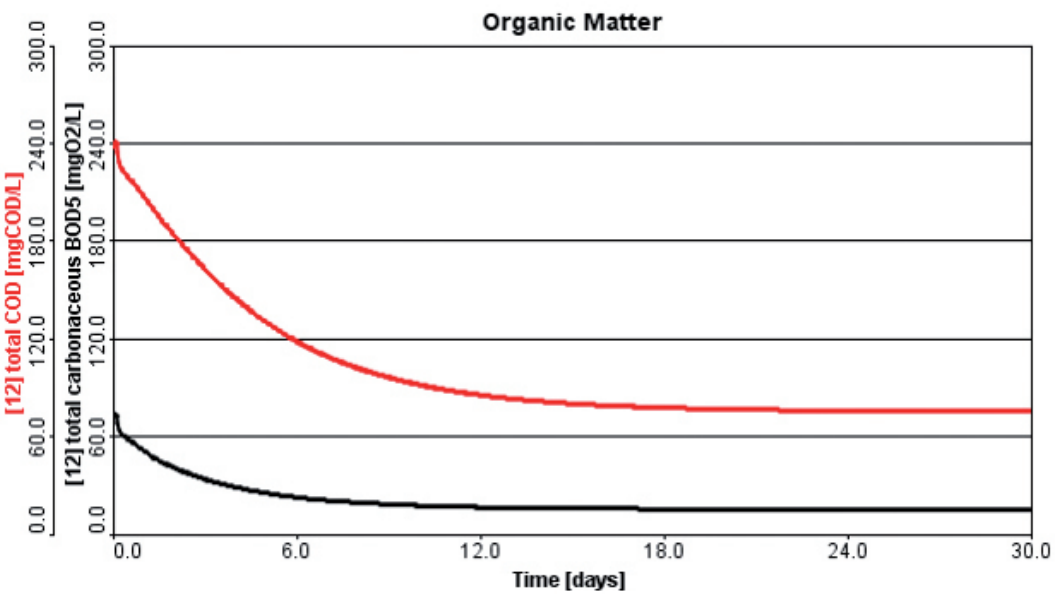

Figure 15
Treated effluent COD and BOD_5 (compiled by the author)

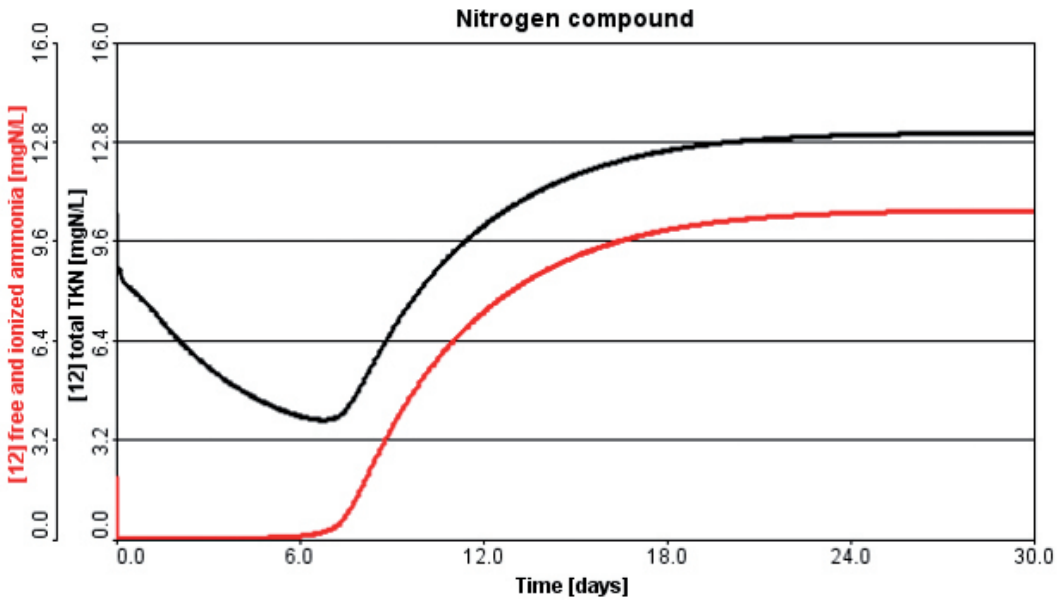

Figure 16
Treated effluent nitrogen compounds (compiled by the author)

Effluent nitrogen concentrations stabilised after 15–18 days. Organic nitrogen is about 3 mg/l and ammonium-nitrogen is about 9 mg/l. With aeration control, further fine tuning is possible.

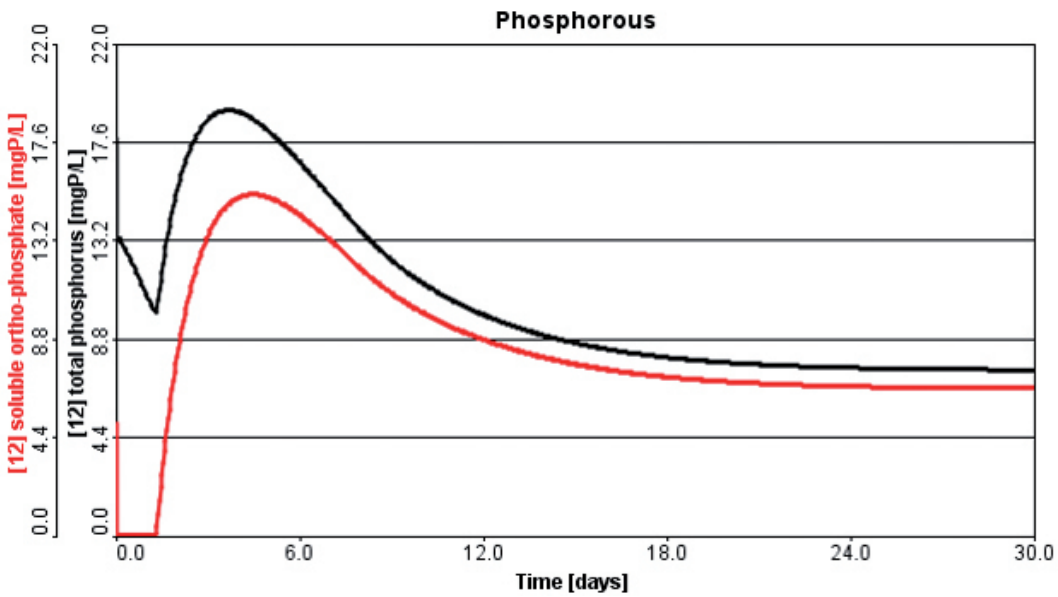

Figure 17
Effluent phosphorus concentration (compiled by the author)

For phosphorous forms, the ratio of orthophosphate/total phosphorus in treated wastewater is high. We could remove as much phosphorus as the biomass would take. It follows that if a higher degree of nutrient removal is desired, chemical precipitation is essential.

SBR system

With batch reactors, high treatment efficiency can also be achieved. The essence of the technology is that instead of spatial separation of the reactor zones, time cycles are applied and the entire treatment process takes place in one basin. This means that cycles that are usually 6–8 hours long can be divided into the following processes:

- feed
- biological processes (mixing and aeration or mixing without aeration)
- sedimentation
- decanting

The steps and cycle times should be designed in such a way that an entire number of cycles take place in one day. The general rule of thumb is that the feed is approximately half an hour, the settling is 1.2–1.5 h, decanting is minimum half an hour. The rest of the time has been developed for biological processes. The mixing and aeration time creates aerobic conditions, the mixing but non-aerating part is anoxic. Separation of individual processes is not necessary. Decantation can also occur simultaneously with the sedimentation supposing the exact knowledge on sludge blanket level changes in the basin.

The design of SBR plants is usually done by the analogy method: the conventional activated sludge technology is scaled and these reactor volumes and ratios are changed over time (using the hydraulic residence time t = V/Q).

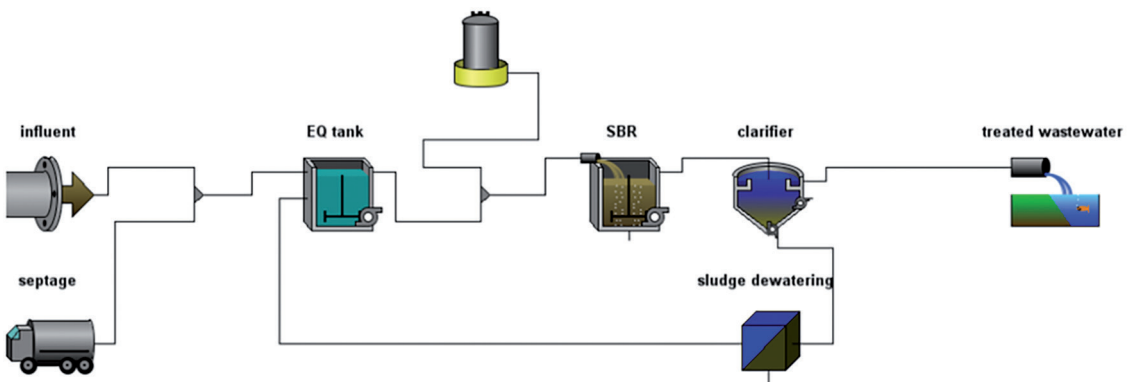

Figure 18
SBR system GPS-X 6.5. model layout (compiled by the author)

Sizing of SBR is also based on mass balance modelling. Here, the input time parameter should be the cycle times in addition to the usual flowrate volume, DO, MLSS, recirculation. When using SBR, you may need to use equalisation basins. The advantage of SBR over the conventional sludge system is:

– easy operation (automation)
– flexibility (you can change cycle times, operating volume cannot be changed)
– better settling sludge
– higher allowable MLSS concentration
– relatively small space requirement

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Questions

1. What is the difference between a model and a simulator?
2. What are the basic processes for building an activated sludge model?
3. What input parameters are required for a mass balance modelling for fixed carrier systems?
4. Describe the Takács sedimentation model!
5. Define AOTR and SOTR! What is the relationship between them?
6. Describe the PID control logic!
7. What kind of ideal reactor models do you know?
8. What are the effects of recirculation in wastewater treatment technologies on the reactor model?
9. What is virtual reactor number?
10. How does cascading affect sludge production?
11. How does the model layout of a small wastewater treatment unit look like?
12. What simulation steps should be taken in mass balance modelling of small treatment units?
13. What can you say about SBR systems?