CFD Simulation of biochemical processes and experimental comparison in an activated sludge aeration tank

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Abstract

With the objective to increase the efficiency of the aeration tanks of municipal wastewater treatment plants, the present work deals with the complete and systematic coupling of a biological model system with a commercial CFD Code, ANSYS CFX . In addition to the implementation of appropriate biological processes, the modeling of a three-phase flow, mass transport and rheology of activated sludge are presented and validated by experimental data. Effects of parameter variations on the simulation quality are examined and a comparison with indus-trial standard simulation-tools is performed. Besides the simulation of test geometries, illustrating the general functionality of the model, the simulation of a real aeration tank will be presented so that an assessment of the quality of the simulation can be performed. Experiments are carried out at a sewage treatment plant to determine concentration profiles for verification. Results show that the model beats common simulation standards in its accuracy. For the investigation of critical factors affecting the overall simulation, a sensitivity analysis of key parameters is performed. Lastly, conclusions for possible optimization mare proposed based upon the simulation results. **Keywords** CFD; activated sludge; biological reactions, viscosity, oxygen transfer

INTRODUCTION

As demands on the cleaning performance of wastewater treatment plants (WWTP) in densely populated areas increase steadily, economic interests must be taken into account at the same time. More than 60% of the total energy consumption of wastewater treatment plants falls on the aeration of activated sludge, which is usually used in most of these plants. Oxygen is required to provide the microorganisms. This contributes to a significant part of the operating costs. Obviously, the optimization in this area can have an immense effect, by only applying minor modifications. Within the reactor mass transfer limitations and hydrodynamics play an important role, since bacteria use dissolved oxygen, carbon and nitrogen in the wastewater as a food source. Biochemical processes within the reaction volume can be described using the "Activated Sludge Model No.1 (ASM1)", published in the Scientific and Technical Report No. 9 of the IWA by Henze et al. (2000). This model is widely used in systemic 0D simulation programs for process control. It provides the biological kinetics models that predict mathematically the carbon oxidation, nitrification and denitrification of pollutants in waste water but it lacks a sufficient mass transfer model. Coupling the main biochemical processes with appropriate hydrodynamics inevitably leads to the use of CFD for high-resolution 3D simulations. The visualization of biological processes, mass transfer limitations and hydrodynamics within the reactor can reveal untapped potential for optimization. One possible optimization method could be the installation of suitable mixing devices or the rearrangement of aerator patterns.

However, it has not been possible to obtain a satisfying forecast for all parameters involved in the effluent, in particular for the nitrate concentration. To achieve this goal, further modeling is still required, but as the complexity increases processing power must be considered simultaneously.

METHODS

CFD simulation setup

All presented modeling results were implemented into the commercial code ANSYS CFX 13.1, by means of user defined functions. Because of the high gas loads in the liquid phase, we have used an Euler-Euler approach with two distinct Euler phases. A liquid continuous phase and a dispersed gas phase with a bubble diameter of 3 mm was established. The suspended solids components derived from the ASM1 are implemented into the liquid phase and affected by the "algebraic slip model". Hence, a relative movement of the insoluble components within the continuous phase could be achieved. Simulations were carried out on workstations running on 4 cores at 3.1 GHz.

Settling of activated sludge

Data for the estimation of settling velocities v_s were collected from secondary clarifier experiments by Janzen (2005) and taken from Schumacher (2006). They were used for the modeling and compared to simulations as they depend on the TSS. Tacàcs (2008) suggested a modeling approach that subdivides the settling of the activated sludge into two linear and one exponential region illustrated in Fig. 1 and described in Table. 1.

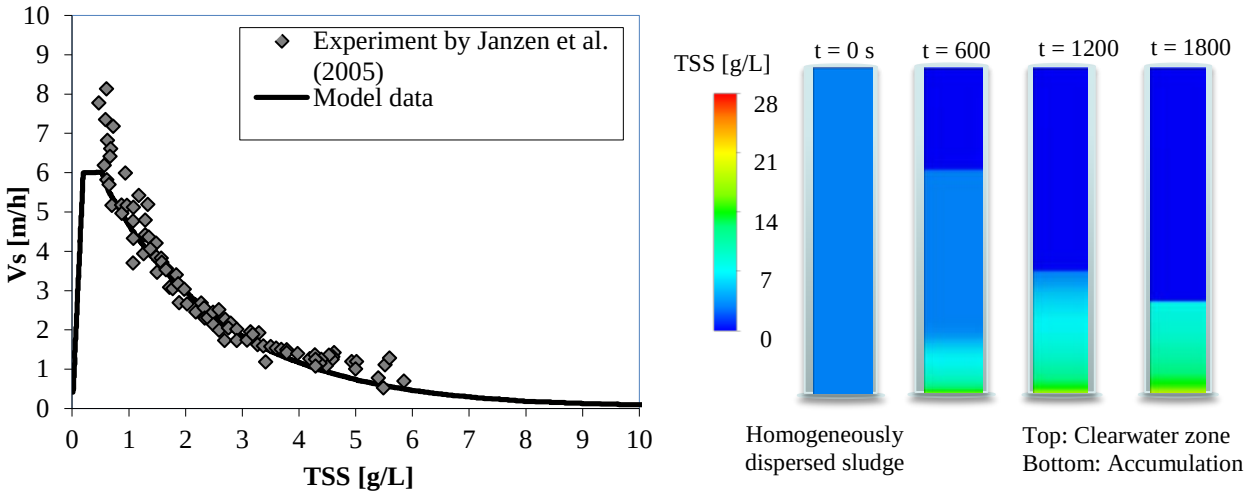

Fig. 1. Experimental settling velocity vs. suspended solids (left) and sedimentation simulations in virtual graded cylinders with a homogenously dispersed initial condition of TSS = 3 g/L (right).

Ordinary activated sludge aeration tanks usually work with TSS > 2 g/L, so that the focus is put on the double exponential Eq. (3) for TSS > 0,476 kg/m^3 as suggested by Takács et al. (1991). Model fitting for the settlement data gathered by Janzen et al. (2005) was carried out with the Excel Solver by means of least squares method.

Table 1. Mathematical modeling of experimental sedimentation data.

Total suspended solids [kg/m³]	Settling velocity [m/h]	
0 – 0,2	$v_s = 31{,}283\left[\frac{m^4}{kg \cdot h}\right] \cdot TSS$	(1)
0,2 – 0,476	$v_s = 6\left[\frac{m}{h}\right]$	(2)
> 0,476	$v_s = 7{,}443\left[\frac{m}{h}\right] \cdot \left(e^{\left(-0{,}4628\left[\frac{m^3}{kg}\right] \cdot TSS\right)} - e^{\left(-25{,}005\left[\frac{m^3}{kg}\right] \cdot TSS\right)}\right)$	(3)

Eq. 1-3 are used by the algebraic slip model in ANSYS CFX. The equations are triggered for each computational grid cell by TSS and affect all insoluble ingredients considered to belong to an activated sludge floc, e.g. heterotrophic and autotrophic biomass. The relative settling velocity is directed towards ground, superimposing gravity and buoyancy. For turbulence modelling the SST-Model approach is used

Modeling of activated sludge viscosity

Schumacher (2006) and Oertel et al. (2009) showed, that the viscosity of the activated sludge can be described as a combination of Newtonian and Bingham fluid. The Newtonian character of the fluid can be found at lower TSS and smaller shearing rates while a Bingham behavior can be observed at higher TSS. This phenomenon is illustrated in a shear stress diagram on the left side of Fig. 2.

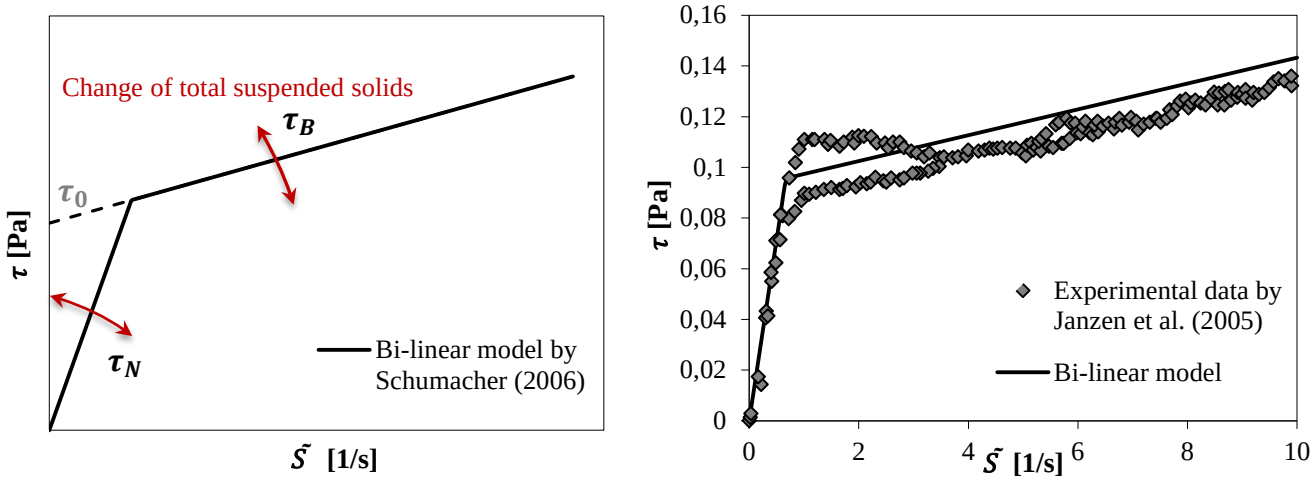

Fig. 2 Bi-linear viscosity behavior of activated sludge as a function of TSS and shear rate (left) as proposed by Schumacher (2006). Experimental data could be successfully described with this model approach (right).

Depending on TSS and the shear rate $\tilde{S}$, either the Newtonian approach τ_N or the Bingham approach τ_B for the shear stress is chosen. Resulting viscosity is represented by a minimum function which is shown in Eq. 4.

$$\eta = \frac{Min(\tau_N, \tau_B)}{\tilde{S}} \tag{4}$$

The right side of Fig. 2 illustrates experimental and model results, carried out by the bi-linear approach. Equation (5) describes the algebraic mathematical modeling of the viscosity with respect to TSS and the viscosity of water η_w:

$$\eta = \frac{Min\left(\left\{\left(\boldsymbol{K_1}\cdot DM^2 + \eta_w\right)\cdot\tilde{S}\right\}, \left\{\left(\boldsymbol{K_3}\cdot DM^3 + \boldsymbol{K_4}\cdot DM\right) + \left(\boldsymbol{K_2}\cdot DM^2 + \eta_w\right)\cdot\tilde{S}\right\}\right)}{\tilde{S}}. \tag{5}$$

The constants K_1- K_4 listed in Tab. 2 have been fitted to various published viscosity plots for several TSS as presented in Fig. 2.

Table 2. Empirical fitted constants of Eq. 5

$K_1 = 0{,}00348\left[\frac{m^5}{kg \cdot s}\right]$	$K_3 = 0{,}00023\left[\frac{m^8}{kg^2 \cdot s^2}\right]$
$K_2 = 0{,}00010\left[\frac{m^5}{kg \cdot s}\right]$	$K_4 = 0{,}00488\left[\frac{m^2}{s^2}\right]$

Oxygen transfer modeling

A two-film model approach is used for the description of the interphase transfer between gas and liquid phase. The concentration profile inside the gas bubbles is neglected and the interfacial gas phase concentration is calculated by Henry's law.

As described by Higbie (1935) and Wagner (1991) the, liquid phase oxygen transfer coefficient K_L depends on diffusion coefficient D_L, the bubble diameter $d_{B,}$ and the rising velocity of the bubble v_S:

$$k_L = 2 \cdot \sqrt{\frac{D_L \cdot v_S}{\pi \cdot d_B}} \tag{6}$$

The latter can be related to liquid dynamic viscosity η_L and density ρ_L and described as follows:

$$v_S = \left(\frac{g^3 \cdot {d_B}^5 \cdot {\rho_L}^2}{2209 \cdot {\eta_L}^2}\right)^{0{,}25} \tag{7}$$

$$D_L = \frac{1}{3 \cdot \pi \cdot d_{O_2} \cdot \eta_L} \cdot \frac{R \cdot T}{N_A} \tag{8}$$

with additional variables for the gravity constant g, the ideal gas constant R the Avogadro constant N_A, temperature T and the diameter of an oxygen molecule d_{O2}.

Consequently, this results in a modified Higbie's film penetration theory suggested by Krause (2001) according to Eq. 9

$$k_L = \frac{2}{\pi} \cdot \sqrt{\frac{R \cdot T \cdot g^{0{,}75} \cdot {d_B}^{0{,}25} \cdot {\rho_L}^{0{,}5}}{3 \cdot N_A \cdot d_{O_2} \cdot {\eta_L}^{1{,}5} \cdot 2209^{0{,}25}}}\ , \tag{9}$$

which has been finally implemented into the CFX code.

Implementation of the Activated Sludge Model No.1

ANSYS CFX is not capable of handling mass-based systems like the ASM1 by itself. The ASM1 model was, therefore, converted into a molar based system. IWA standard advised values for all process components and half-saturation coefficients have been used and were taken from Henze et al. (2000). To put them on a molar basis, they have been divided by suitable molar masses. Mass based kinetic reaction rates of the Matlab calculations had to be fitted via differential quotients by the Excel Solver and brought to consistency. Finally, eight molar based reactions together with their appropriate kinetic parameters have been implemented into CFX.

As calculations of the ASM1 in Matlab are not influenced by any mass

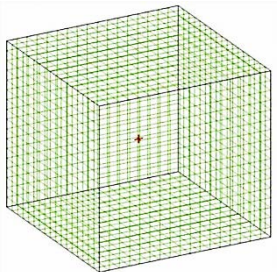

Fig. 3. Test geometry for CFX outputs

transfer limitations, we used a perfect cube geometry (Fig. 3) in CFX without any hydrodynamic effects such as turbulence modeling or mass transfer limitations. Consequently, the geometry can be regarded as continuous stirred-tank reactor. Considering the same initial conditions, simulations are carried out with equal start values for each component of the ASM1 model in Matlab and CFX. Oxygen concentration is considered to be fixed with a concentration of 6 mg/L. Only one single Euler phase is implemented. The cross in the middle of the geometry indicates the measuring point where simulation data are gathered.

Experiments

Figure 4 shows the aeration Sludge Samples were taken hourly at the measurement points S1-S7 and half-hourly at the influent point (S0). They were instantly analysed for chemical oxygen demand (COD), ammonia- (NH_4-N) and nitrate – nitrogen (NO_3-N) by photometric rapid test.

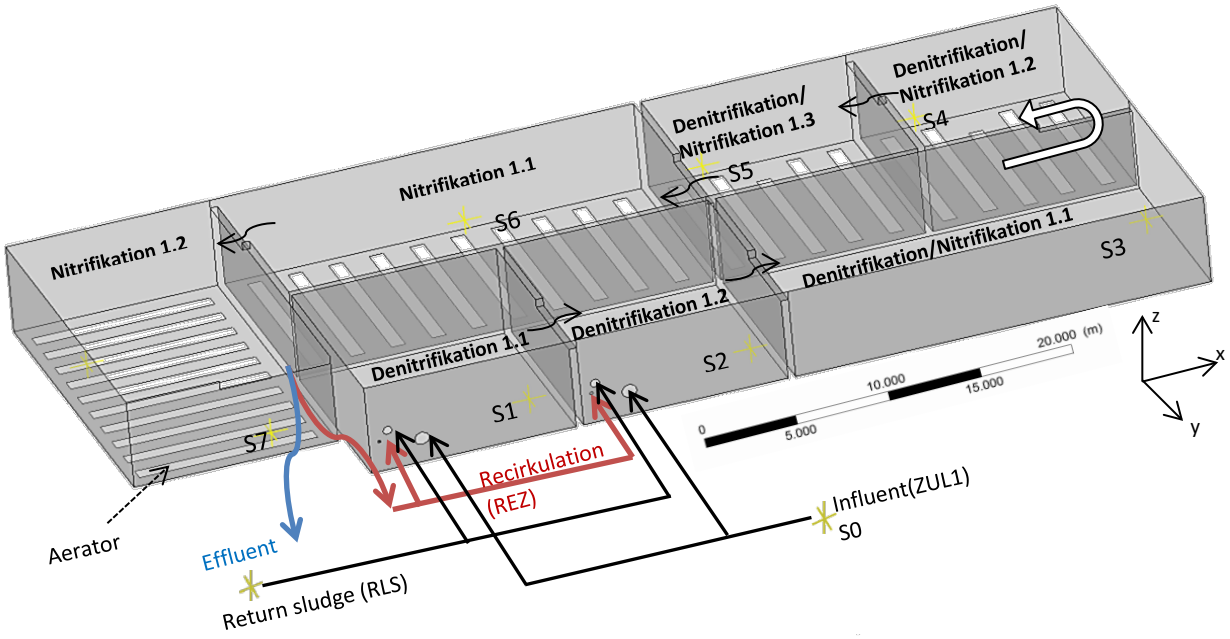

Fig. 4. Aeration Tank of a municipal waste water treatment plant used for experimental verification.

RESULTS AND DISCUSSION

Simulation of settling and viscosity

Simulations of settling velocity and viscosity are compared to experimental model data. Fig. 5 shows good agreement of the simulations carried out in virtual rotary disk viscometers and experiments.

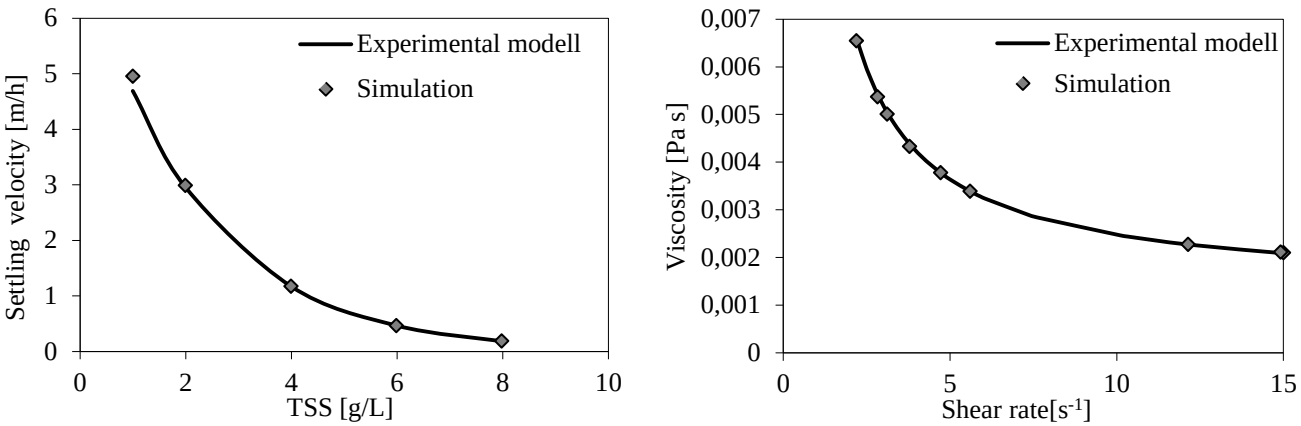

Fig. 5. Simulation results of activated sludge settling (left) and viscosity (right)

Experimental model data are compared to sedimentation simulations in virtual graduated cylinders, which is also common experimental practise for the estimation of sludge volume (left side of Fig. 5). The plot shows the successful adaption of the experimental values. The SST model by Menter (1994) is used for turbulence modeling as it reveals crucial relevance: Due to the wall effects, best results are obtained with it in comparison to other turbulence models. Stobbe (1964) has already described these wall effects in his experimental setup for sludge level estimation.
Viscosity simulations in virtual shearing disc viscometers are compared to the experimental data (right side of Fig. 5). Simulation and experimental model show only minor discrepancy. The viscosity and settling rate of the activated sludge within the liquid Euler phase can, therefore, be regarded as successfully implemented.

Comparison of molar and mass based simulations

Simulations of Matlab and ANSYS CFX calculations are shown in Fig. 6. The CFX calculations were carried out with fitted parameters for the specific growth rate and decay of heterotrophs μ_H, b_H / autotrophs μ_A, b_A, hydrolysis rate k_h and ammonification rate k_a on a molar basis. All graphs show logical trends and good congruency of both solver runs for each component of the implemented reactions. Thus, fitting and implementation of kinetic constants into CFX can be stated as successful. One should keep in mind that these simulations do not consider mass transfer characteristics.

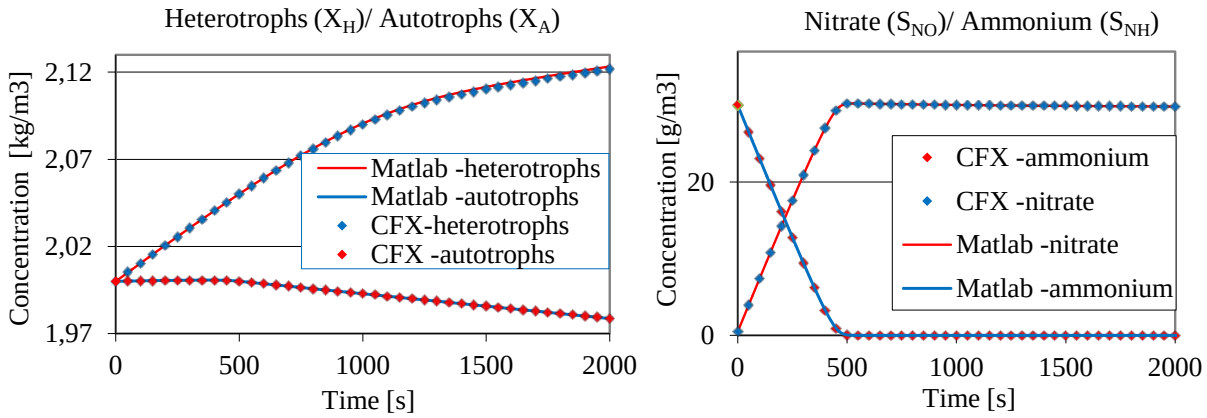

Fig. 6. Simulation outputs of main ASM1 processes in mass based Matlab and molar based CFX calculations

Simulation results

Bio-kinetics coupled CFD simulations have been carried out in several test geometries. Fig. 7 shows a half aerated channel with wastewater inflow from the left side and outlet on the right. The simulations are steady state simulations containing the previously described models. Nitrate concentration plots on the left of Fig. 7 shows an expected behaviour of the degradation. It can be viewed as an example component taken from the ASM1. In the aerated zone, nitrification takes place whereas the un-aerated part advances the denitrification, i.e. nitrate degradation. Non aerated areas show less turbulence than at the beginning of the channel which contains the sparging components. Sedimentation and accumulation takes place in the less turbulent zones. The right side of Fig. 7 is showing exemplarily the sedimentation of organic solids in the non-aerated zone.

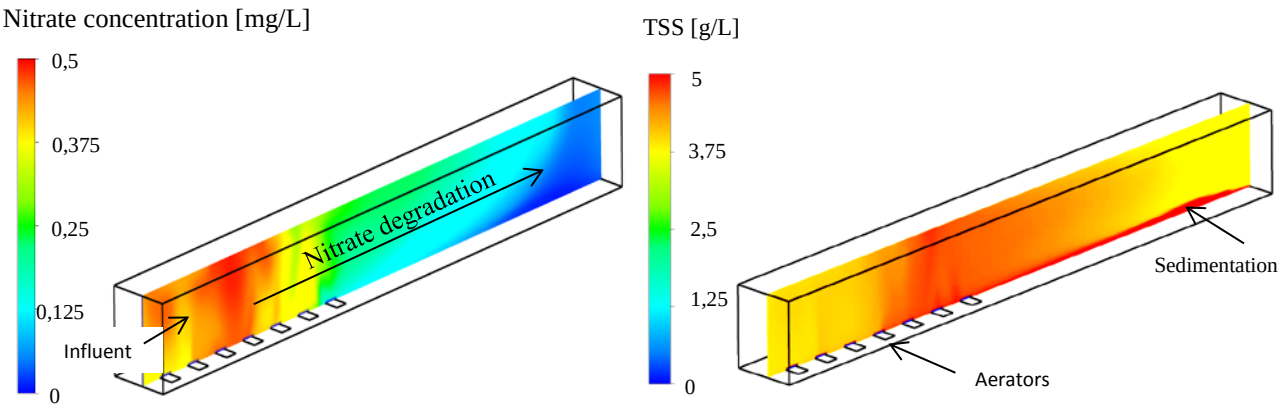

Fig. 7. Nitrate concentration (left) and sedimentation in a partly aerated channel Testgeometry

The sedimentation in the aeration tank is negligible as shown in .Fig. 8. It seems that turbulence far outweighs sedimentation. Sludge velocity on the ground of the tanks reaches 30 cm/s which can be seen to be fairly high. It should be considered to remove mixing devices in aerated zones to save energy.

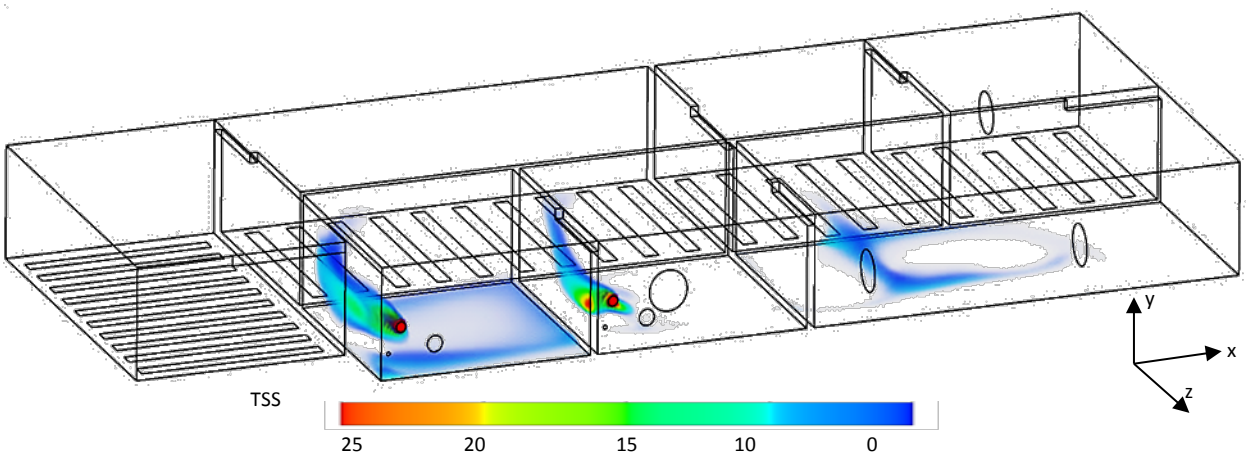

Fig. 8. Simulation results for the sedimentation within the activated sludge tank.

Simulation vs. experimental concentration profiles are shown in Fig. 9 for hourly measurements. It can be seen that the experimental curve is well represented by the simulation and the bulk of the simulated values is within the error range of the measurements. At the same time it must be noted that the reduction of nitrate is slightly overestimated in the aerated zones. Since the same is true for the simulation of the ammonia, the conclusion suggests that either the substrate kinetic is overestimated or a wrong ratio of living to inert biomass causes the high turnover rates.

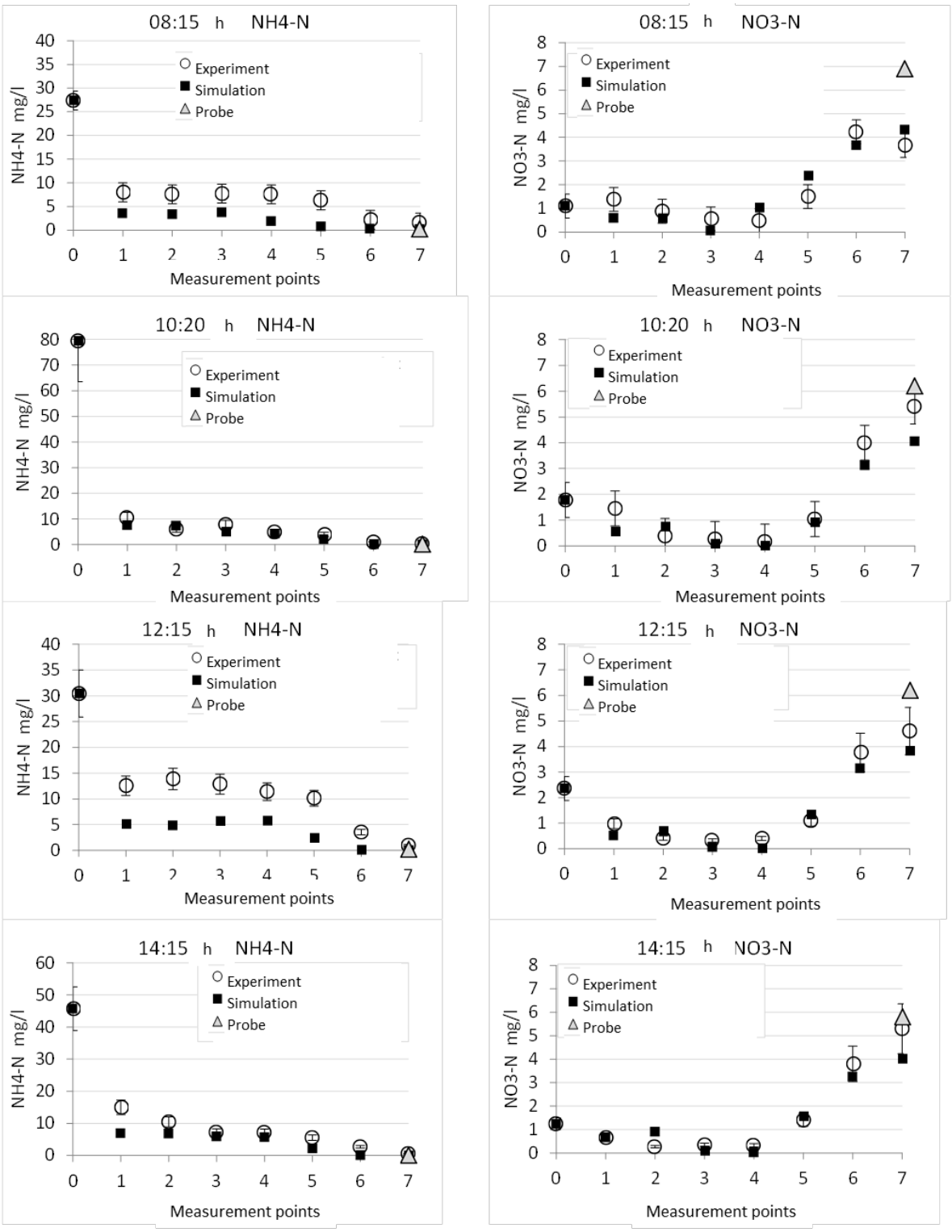

Fig. 9. Concentration profiles within the activated sludge tank. Experimental and simulation results in comparison.

CONCLUSIONS

Modeling approaches of activated sludge have been presented. Literature data from activated sludge experiments in secondary clarifiers were used to model the rheological behaviour of activated sludge. Models were implemented into the commercial CFD code ANSYS CFX and simulations for test geometries were carried out. Although only a two phase Euler-Euler model was considered,

simulations show good accordance to the experimental outcomes. By using algebraic equations, superposing the velocity field of the liquid phase, we could attain sedimentation of the biomass and save calculation power in contrast to a three-phase Euler approach. The implemented viscosity model gave us the opportunity to calculate the mass transfer coefficient K_L in relation to the suspended solids and shear rates. Moreover, it was possible to put the mass based ASM1 model on a molar basis with fitted kinetics parameters, allowing the implementation into CFX. The implemented models will give a more detailed view on a simulated geometry and are able to reveal zones where sludge settling takes place. Thus, oxygen transfer into the activated sludge can be calculated by this approach. Simulated test geometries are presented and showed logical and expected behavior of the simulated degradation process.
Simulations of the activated sludge tank show a discrepancy between experimental measurements in ammonia and nitrate concentration to experimental data that is possibly due to a wrong ratio of living to inert biomass in the ASM1. It can be stated that microbiological batch experiments are most important for the estimation of the correct biomass ratio between heterotrophs and autotrophs.

REFERENCES

Gresch M., Brugger R., Meyer A. and W. Gujer (2009). Compartmental Models for Continuous Flow Reactors Derived from CFD Simulations. *Environmental Science & Technology* 43(7): 2381-2387.

Henze M., Gujer W., Mina T. and M. C. M. van Loosdrecht (2000). *Activated Sludge Models ASM1, ASM2, ASM2D and ASM3*. Scientific and Technical Report series. London, IWA Publishing.

Higbie R. (1935). The rate of absorption of a pure gas into a still liquid during short periods of exposure, *American Institute of Chemical Engineers*, 31, (65), 365-389.

Janzen M. and K.-H. Rosenwinkel (2005). *Verbesserung der Gestaltung von Zu- und Abläufen bei horizontal durchströmten runden Nachklärbecken (Improving the design of inlets and outlets for horizontal flow in round settling tanks),* Report, University of Hannover.

Le Moullec Y., Gentric C., Potier O. and J. P. Leclerc (2009). Comparison of systemic,compartmental and CFD modelling approaches: Application to the simulation of a biological reactor of wastewater treatment. *Chemical Engineering Science*.

Le Moullec Y., Potier O., Gentric C. and J. P. Leclerc (2011). Activated sludge pilot plant: Comparison between experimental and predicted concentration profiles using three different modelling approaches. *Water Research* 45: 3085-3097.

Menter F. R. (1994). Two-Equation Eddy-Viscosity Turbulence Models for Engineering Applications. In: AIAA, J., vol. 32, no 8. pp. 1598-1605.

Oertel H. j., Böhle M. and U. Dohrmann (2009), *Strömungsmechanik (Fluidmechanics)*, 5th edt., Vieweg und Teubner GWV Fachverlage GmbH, Wiesbaden.

Schumacher S. (2006). *Leistungsbestimmende Prozesse in Nachklärbecken - Einflussgrößen, Modellbildung und Optimierung (Performance determining processes in clarifiers – Influencing variables, modeling and optimization).* PhD thesis, Institute of Fluid Mechanics and Environmental Physics in Civil Engineering, University of Hannover.

Stobbe G. (1964). *Über das Verhalten von belebtem Schlamm in aufsteigender Wasserbewegung (About the behavior of activated sludge in an ascending water movement)* ; Report, Institute for Water Quality and Waste Management,University of Hannover; Nr. 18; Hannover.

Takács I., Patry G.G. and D. Nolasco (1991) A Dynamic Model of the Clarification – Thickening Process. *Water Research* 25(10).

Takács I. (2008) *Experiments in Activated Sludge Modelling*. PhD thesis, University of Ghent.

Wagner M. (1991). *Einfluss oberflächenaktiver Substanzen auf Stoffaustauschmechanismen und Sauerstoffeintrag (Influence of surfactants on mass transfer mechanisms and oxygen)* PhD thesis, IWAR Institute, Technical university of Darmstadt.