



ADAPTATION OF THE *SIMPLETREAT* CHEMICAL FATE MODEL TO SINGLE-SLUDGE BIOLOGICAL NUTRIENT REMOVAL WASTEWATER TREATMENT PLANTS

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ABSTRACT

Many recent developments in municipal waste water treatment technology are directed towards biological nutrient removal. Chemical fate models which are used to predict the behavior of individual chemicals in waste water treatment plants (WWTPs), have until now not incorporated this aspect. In this paper, two modifications to the steady-state non-equilibrium *SimpleTreat* modeling concept (Struijs *et al.*, 1991; Struijs, 1996) are presented. These focus on an improved description of sludge recycling, and on the presence of different redox zones in the biological reactor (aerobic, anoxic, anaerobic). The updated models were applied to three different WWTP designs, and simulation results were compared to measured values for the surfactant LAS. © 1998 Elsevier Science Ltd. All rights reserved

KEYWORDS

Biological nutrient removal; CAS unit; Chemical fate; LAS; *SimpleTreat*; UCT process

INTRODUCTION

For environmental risk assessment of chemicals, accurate exposure predictions are required (e.g. ECETOC, 1994). An important factor which determines aquatic exposure to 'down-the-drain' chemicals is their degree of elimination in WWTPs. To predict such removal efficiencies, several chemical fate models have been developed (e.g. Blackburn and Troxler, 1984; Namkung and Rittmann, 1987; Govind *et al.*, 1991; Struijs *et al.*, 1991; Cowan *et al.*, 1993; Melcer *et al.*, 1994; Jacobsen *et al.*, 1996; Struijs, 1996; McAvoy *et al.*, 1997). The existing steady-state WWTP fate models are typically based on 'standard' plant configurations, designed in first instance for carbon removal. However, nowadays biological nutrient removal has become an important aspect in municipal waste water treatment and water quality management (e.g. CEC, 1991). Many WWTPs in Europe are upgraded to include nitrogen and phosphorus removal, or will be in the near future. Hence, it is warranted to include the effect of nutrient removal processes on chemical fate. In this paper, a modification of the *SimpleTreat* model is presented, which describes chemical fate (as parent removal) in typical single-sludge biological nutrient removal WWTPs. In the modified model, an improved description of sludge recycling is used, and the presence of different redox zones is taken into account.

MODELING APPROACH

The current state of the art in steady-state WWTP fate models is mainly represented by *TOXCHEM* (Melcer *et al.*, 1994), *AS-TREAT* (McAvoy *et al.*, 1997), and *SimpleTreat* (Struijs *et al.*, 1991; Struijs, 1996). The latter was chosen as a starting point for the development of a nutrient removal plant model, because of the inherent flexibility of its fugacity approach, and because of its regulatory acceptance within European Union risk assessment.

In the *SimpleTreat* approach, a WWTP is represented by a number of compartments (boxes). Each chemical phase in each reactor is assigned one box. A standard carbon removal plant (without considering primary settling) consists of 6 boxes: air above the WWTP, dissolved and sorbed chemical in the activated sludge tank, dissolved and sorbed chemical in the settler, and sorbed chemical in the settled sludge. Mass balancing for all boxes is performed using the *SIMPLEBOX* method (van de Meent, 1993). At steady-state, the equation for each box i is:

$$k_i \cdot C_i \cdot V_i + \sum_{j=1}^6 (ADV_{i,j} + XCH_{i,j}) \cdot C_j + ADV_{i,0} \cdot C_i - \sum_{j=1}^6 (ADV_{j,i} + XCH_{j,i}) \cdot C_j = \Phi_{in}^i$$

| | | | |
|------|---------------|---|----------|
| with | k_i | chemical elimination rate in box i | s^{-1} |
| | $ADV_{i,j}$ | advective transport volume flux from box i to j | m^3/s |
| | $XCH_{i,j}$ | diffusive exchange volume flux from box i to j | m^3/s |
| | C_i | chemical concentration in box i | g/m^3 |
| | V_i | volume of box i | m^3 |
| | Φ_{in}^i | chemical influx from out of the system into box i | g/s |

Finally, the concentrations in each box (C_i) are obtained by solving the set of mass balance equations through matrix inversion. Note that transport to or exchange with other boxes is described by the advection and exchange terms. Both are expressed as media volume flows, where the medium can be air, water or solids. The exchange terms are calculated from chemical diffusion coefficients between boxes ($D_{i,j}$) and the chemical fugacity in each box (Z_i) (after Mackay and Paterson, 1982).

NUTRIENT REMOVAL PLANT CONFIGURATION

For development of the fate model, the University of Capetown (UCT) reactor design was chosen (Ekama *et al.*, 1984). A UCT plant consists of three activated sludge tanks (or zones) in sequence: anaerobic, anoxic and aerobic. Sludge is recycled internally between the aerobic and the anoxic tank, and between the anoxic and anaerobic tank. Settled sludge is recycled to the anoxic tank. Many other plant designs are basically identical to this scheme (Henze, 1996), or can be simplified to fit into it. Note that sequential batch reactors (SBR) can also be represented in this framework, using hypothetical volumes derived from the fraction of time taken by the different redox stages.

SLUDGE RECYCLING

In *SimpleTreat*, only the solids phase of the recycled sludge is considered. Moreover, different sludge recycle flows and recycling ratios cannot be taken into account. As in nutrient removal processes sludge recycling is crucial, the effect of including a more realistic description of these recycles into the *SimpleTreat* concept was explored.

Modifications to the *SimpleTreat* Model

The modified recycle flows are illustrated below in Figure 2. It was assumed that the interstitial water phase of the settled sludge is identical to the main water phase in the settler (box 4). Hence, the water phase of the sludge recycle could be represented by an advective transport of settler water to the activated sludge tank ($ADV_{4,2}$). The activated sludge tank's flow balance was corrected for this additional inflow, by modifying the term $ADV_{2,4}$. To take into account the actual recycle flow of the solids phase, the $ADV_{3,5}$ term was also updated.

| | water phase | solids phase |
|--------------------------|-------------------------------|--|
| plant in-/outflow: | $ADV_{0,2} = Q$ | $ADV_{0,3} = Q \cdot SS_{sewage} / \rho_{solids}^{sewage}$ |
| | $ADV_{4,0} = Q$ | $ADV_{5,0} = Q \cdot SS_{effluent} / \rho_{solids}^{ML}$ |
| sludge propagation: | $ADV_{2,4} = Q \cdot (1 + R)$ | $ADV_{3,5} = Q \cdot (1 + R) \cdot SS_{ML} / \rho_{solids}^{ML}$ |
| settled sludge recycle: | $ADV_{4,2} = Q \cdot R$ | $ADV_{6,3} = ADV_{5,6} - ADV_{6,0}$ |
| sludge settling + waste: | | $ADV_{5,6} = ADV_{3,5} - ADV_{5,0}$ |
| | | $ADV_{6,0} = \Phi_{surplus}^{SS} \cdot 1 / \rho_{solids}^{ML}$ |

| | | |
|-------------------------------------|--|-----------------------|
| with Q | WWTP influent flow | m^3/s |
| SS_x | suspended solids level in compartment x | g/m^3 |
| ρ_{solids}^x | density of solids in compartment x | g/m^3 |
| R | recycle ratio | - |
| $\Phi_{\text{surplus}}^{\text{SS}}$ | surplus mixed liquor solids flux (which is to be wasted) | g/s |

Sensitivity of Chemical Fate Predictions to the Recycle Ratio

Theoretical Considerations

Chemical Concentrations: The chemical concentration entering the settler is identical to the completely mixed activated sludge tank concentration. In the settler, volatilization causes further elimination of the dissolved chemical. Hence, for volatile chemicals, the dissolved concentration in the settler is expected to be lower than that in the activated sludge tank. As a result, recycling of the settler's water phase will have a (relatively small) diluting effect on the latter.

Hydraulic Residence Time: The hydraulic residence time in the activated sludge tank is decreased by including a water recycle flow. However, the average total residence time is not affected, as the recycling causes multiple passes through the tank.

Expected Effects: (1) For chemicals with low volatility, it is expected that the dissolved phase concentration in the settler and in the activated sludge tank are very similar. Hence, the water phase recycle will have a negligible effect on the concentration in the activated sludge tank. As the net residence time in the tank is also not affected, it is expected that the water recycle will have very limited effect on chemical elimination. (2) Volatile chemicals are expected to have a lower dissolved concentration in the settler than in the activated sludge tank. Hence, recycling water will cause a dilution of the latter's dissolved phase, affecting several fate processes. There will be desorption from the solids phase, due to the increased concentration gradient. Consequently, a larger chemical fraction will be available for volatilization and dissolved phase degradation. Hence, it is expected that chemical elimination will be increased.

Simulation

To illustrate these points, the fate of four hypothetical chemicals in the default *SimpleTreat* WWTP configuration was simulated, using different sludge recycle ratios. The four chemicals are Hypotheticum (the default *SimpleTreat* substance), A (sorbing, degradable in the dissolved phase and non-volatile), B (as A, but also degradable in the sorbed phase) and C (sorbing, non-degradable and highly volatile). The properties of these chemicals are given in Table 1.

Table 1. Chemical properties of hypothetical substances

| | K_d sewage (L/kg) | K_d mix. liquor (L/kg) | $k_{\text{degradation}}$ (h^{-1}) | degradation phase | Henry coeff. ($\text{Pa}\cdot\text{m}^3\cdot\text{mol}^{-1}$) |
|--------------|------------------------|-----------------------------|---|----------------------|--|
| Hypotheticum | 300 | 370 | 0.1 | dissolved | 1 |
| Chemical A | 2000 | 2000 | 0.69 | dissolved | 10^{-6} |
| Chemical B | 2000 | 2000 | 0.69 | diss. + sorbed | 10^{-6} |
| Chemical C | 2000 | 2000 | 0 | n.a. | 10^4 |

Sludge recycle ratios were varied between 0 and 3, which represents a realistic range of recycles used in practice for nutrient removal plants. Note that the case with recycle ratio 0 is equivalent to the original *SimpleTreat* setup. In Figure 1, removal efficiencies of the different chemicals were plotted as a function of recycle ratio.

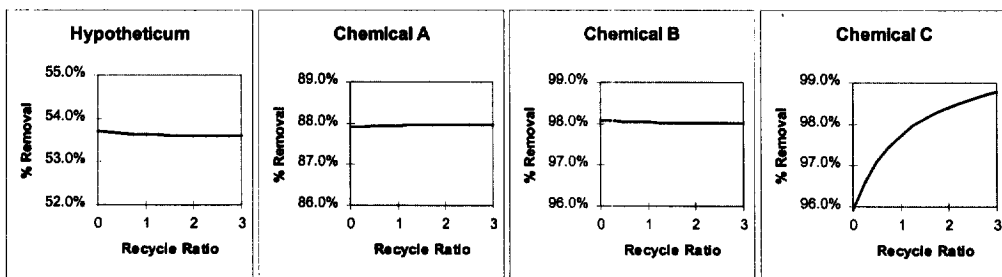


Figure 1. Predicted removal efficiencies as a function of sludge recycle ratio

Discussion

For the low- or non-volatile chemicals Hypotheticum, A and B, the influence of the sludge recycle ratio on chemical elimination was negligible; the absolute difference in predicted removal efficiency was less than 0.1%. For the highly volatile Chemical C, the impact of the recycle ratio was significant. The absolute increase in predicted removal efficiency was approximately 3% when the recycle ratio was varied from 0 to 3. The corresponding decrease in the predicted effluent concentration was a factor 4. This result confirms what was expected from the theoretical considerations above.

MODEL ADAPTATIONS

Two models were developed. The first model is very similar to the original *SimpleTreat* 6-box model. The main modifications are related to sludge recycling and to a correction of the activated sludge tank stripping and degradation rate, based on the presence of different redox zones. The second model is a direct representation of the UCT process, making use of 3 functionally different activated sludge tanks. Here, a 10-box representation is required.

6-box model

The 6-box scheme was derived directly from *SimpleTreat* (Figure 2). The boxes were re-numbered, as in this case no primary settler was modeled. Advective flows were added / modified to obtain a better description of sludge recycling, as described above. The activated sludge tank is split into 3 zones: anaerobic, anoxic and aerobic. Note that in this model description, internal sludge recycles (i.e. between the different redox zones) can not be taken into account. For a detailed description of the model, reference is made to Struijs (1996). The modifications regarding sludge recycling were presented above; the modifications relating to the presence of several redox zones are given below.

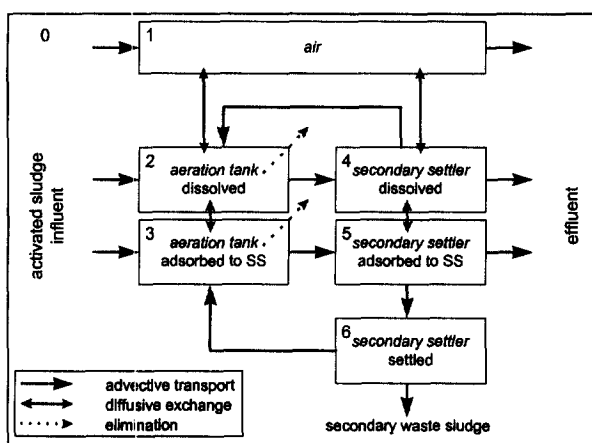


Figure 2. Nutrient removal WWTP fate model - 6-box

Air / Water Exchange

The diffusion coefficients for air / water exchange in the activated sludge tank are calculated as shown below. The surface volatilization term (right) was not changed. In the stripping term (left), both the tank volume and the tank surface area were corrected for the aerobic fraction, finally leading to the aerobic fraction term in the numerator.

$$D_{1,2} = D_{2,1} = \frac{k_{str}}{\frac{1}{V_1 \cdot \frac{(f_{ner}^{AS} \cdot A_{AS})}{A_{total}} \cdot Z_{air}} + \frac{1}{(f_{ner}^{AS} \cdot V_2) \cdot Z_{water}}} + \frac{k_v}{\frac{1}{V_1 \cdot \frac{A_{AS}}{A_{total}} \cdot Z_{air}} + \frac{1}{V_2 \cdot Z_{water}}}} = \frac{f_{aer}^{AS} \cdot k_{str} + k_v}{\frac{1}{V_1 \cdot \frac{A_{AS}}{A_{total}} \cdot Z_{air}} + \frac{1}{V_2 \cdot Z_{water}}}$$

| | | | |
|------|----------------|---|---|
| with | $D_{i,j}$ | chemical diffusion coefficient from box i to box j | $\text{mol} \cdot \text{s}^{-1} \cdot \text{Pa}^{-1}$ |
| | f_{ner}^{AS} | fraction of activated sludge volume which is aerobic | - |
| | k_{str} | 1 st order chemical elimination rate due to stripping | s^{-1} |
| | k_v | 1 st order chemical elimination rate due to surface volatilization | s^{-1} |
| | A_{AS} | surface area of activate sludge tanks | m^2 |
| | A_{total} | total WWTP surface area | m^2 |
| | Z_x | chemical fugacity in compartment x | $\text{mol} \cdot \text{m}^{-3} \cdot \text{Pa}^{-1}$ |

Compared to Struijs (1996), two modifications were made to the calculation of the stripping rate k_{str} . First, the total activated sludge tank volume was replaced by the aerobic volume. Second, the oxygen requirement was adjusted. Additional oxygen input into the aerobic tank is required for nitrification (4.33 mgO₂ per mgN, Metcalf

& Eddy Inc., 1991). On the other hand, oxygen is recuperated thanks to denitrification (2.86 mgO₂ per mgN, Klapwijk, 1978). Uptake of nitrogen into biomass should also be accounted for (here assuming a 5% N-content in biomass).

$$\Delta OxReq = (N - Y \cdot bCOD \cdot 5\%) \cdot (+4.33 \cdot \epsilon_{nitrification} - 2.86 \cdot \epsilon_{nitrification} \cdot \epsilon_{denitrification})$$

| | | |
|---------------------|--|---------------------|
| with $\Delta OxReq$ | adjustment to the oxygen requirement | mgO ₂ /L |
| $bCOD$ | biodegradable chemical oxygen demand in influent | mgO ₂ /L |
| N | nitrogen in influent | mgN/L |
| Y | cell growth yield coefficient | - |
| ϵ_x | conversion efficiency of process x | - |

Chemical Degradation

The chemical degradation rate in the single (mixed) activated sludge tank is calculated as the average of 3 degradation rates, weighted by the residence time in the 3 redox zones. This average rate is obtained from the aerobic degradation rate, by applying the following correction factor:

$$\alpha_{redox} = f_{aer}^{AS} \cdot 1 + f_{anoxic}^{AS} \cdot \alpha_{anoxic} + f_{anaerobic}^{AS} \cdot \alpha_{anaerobic}$$

| | | |
|-----------------------|--|---|
| with α_{redox} | lumped degradation correction factor for different redox zones | - |
| α_x | correction factor for chemical degradation in redox zone x | - |

10-box model

The 10-box model scheme is shown in Figure 3. Each tank was represented by 2 boxes (dissolved and sorbed phase). All possible sludge recycles (from the settler as well as internal recycles) were implemented. Note that in practice only a limited number of sludge recycles are to be selected (as shown in Figure 3 for the standard UCT design). The advective flow terms related to water and solids transport are listed below. The same approach as described above was used to derive these terms.

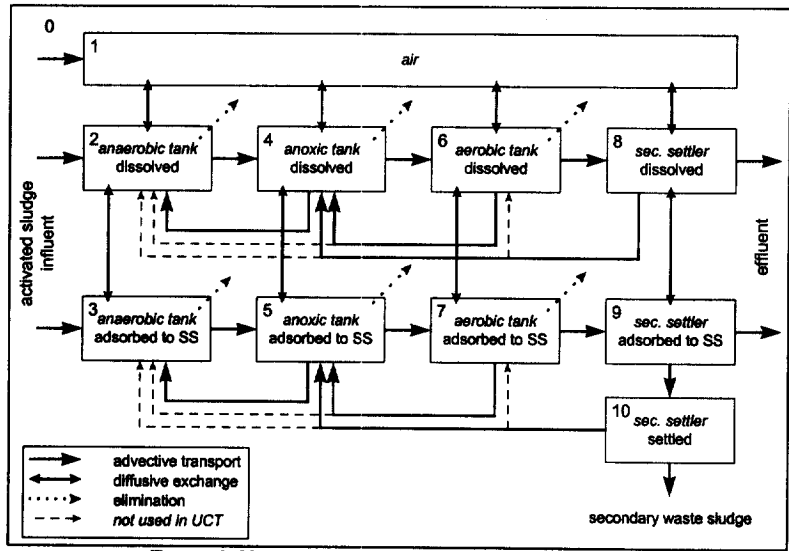


Figure 3. Nutrient removal WWTP fate model - 10-box

| | water phase | solids phase |
|-------------------------|--------------------------------------|---|
| plant in-/outflow: | $ADV_{0,2} = Q$ | $ADV_{0,3} = Q \cdot SS_{sewage} / \rho_{solids}^{sewage}$ |
| | $ADV_{8,0} = Q$ | $ADV_{9,0} = Q \cdot SS_{effluent} / \rho_{solids}^{ML}$ |
| internal recycles: | $ADV_{4,2} = Q \cdot R_{anox,anaer}$ | $ADV_{5,3} = ADV_{4,2} \cdot SS_{anoxic} / \rho_{solids}^{ML}$ |
| | $ADV_{6,2} = Q \cdot R_{aer,anaer}$ | $ADV_{7,3} = ADV_{6,2} \cdot SS_{aerobic} / \rho_{solids}^{ML}$ |
| | $ADV_{6,4} = Q \cdot R_{aer,anox}$ | $ADV_{7,5} = ADV_{6,4} \cdot SS_{aerobic} / \rho_{solids}^{ML}$ |
| settled sludge recycle: | $ADV_{8,2} = Q \cdot R_{S,anaer}$ | $ADV_{10,3} = R_{S,anaer} \cdot \zeta$ |
| | $ADV_{8,4} = Q \cdot R_{S,anox}$ | $ADV_{10,5} = R_{S,anox} \cdot \zeta$ |
| | $ADV_{8,6} = Q \cdot R_{S,aer}$ | $ADV_{10,7} = R_{S,aer} \cdot \zeta$ |

$$\text{with } \zeta = \frac{ADV_{9,10} - ADV_{10,0}}{R_{S,anaerobic} + R_{S,anoxic} + R_{S,aerobic}}$$

| water phase | solids phase |
|--|--|
| sludge propagation: $ADV_{2,4} = Q \cdot (1 + R_{S,anaer} + R_{ner,anaer} + R_{anox,anier})$ $ADV_{4,6} = Q \cdot (1 + R_{S,anaer} + R_{ner,anaer} + R_{anox,anier})$ $+ Q \cdot (R_{S,anox} + R_{ner,anox}) - Q \cdot R_{anox,anaer}$ $= Q \cdot (1 + R_{S,anaer} + R_{S,anox} + R_{ner,anaer} + R_{ner,anox})$ $ADV_{6,8} = Q \cdot (1 + R_{S,anaer} + R_{S,anox} + R_{ner,anaer} + R_{ner,anox})$ $+ Q \cdot R_{S,aer} - Q \cdot (R_{ner,anaer} + R_{ner,anox})$ $= Q \cdot (1 + R_{S,anaer} + R_{S,anox} + R_{S,aer})$ | $ADV_{3,5} = ADV_{2,4} \cdot SS_{anaerobic} / \rho_{solids}^{ML}$ $ADV_{5,7} = ADV_{4,6} \cdot SS_{anoxic} / \rho_{solids}^{ML}$ $ADV_{7,9} = ADV_{6,8} \cdot SS_{aerobic} / \rho_{solids}^{ML}$ |
| sludge settling + waste: | $ADV_{9,10} = ADV_{7,9} - ADV_{9,0}$ $ADV_{10,0} = \Phi_{surplus}^{SS} \cdot 1 / \rho_{solids}^{ML}$ |
| with $R_{i,j}$ sludge recycle ratio from compartment <i>i</i> to <i>j</i> | - |
| $R_{S,i}$ sludge recycle ratio from settler to compartment <i>i</i> | - |

Air / Water Exchange

The diffusion coefficients for air / water exchange in the activated sludge tanks are given below. Surface volatilization is assumed to occur in all tanks, while stripping is assumed to occur only in the aerobic tank. The volatilization rates are calculated by the standard *SimpleTreat* method. The calculation of the stripping rate is similar to the updated 6-box model, also taking into account the adjusted oxygen requirement.

$$D_{1,2/1,4} = D_{2,1/4,1} = \frac{k_v^{2/4}}{\frac{1}{V_1 \cdot \frac{A_{anaer/anox}}{A_{total}} \cdot Z_{air}} + \frac{1}{V_{2/4} \cdot Z_{water}}} \quad D_{1,6} = D_{6,1} = \frac{k_{str} + k_v^6}{\frac{1}{V_1 \cdot \frac{A_{aer}}{A_{total}} \cdot Z_{air}} + \frac{1}{V_6 \cdot Z_{water}}}$$

Chemical Degradation

Separate degradation rates are used for the three tanks (anaerobic, anoxic and aerobic). These are derived from the aerobic rate using the same correction factors as described above for the 6-box model.

MODEL APPLICATION AND CORROBORATION

Description of Treatment Plants and Chemicals

Both models were applied to simulate the fate of Linear Alkylbenzene Sulphonate (LAS), a common surfactant, in three lab-scale activated sludge plants: a standard OECD Continuous Activated Sludge (CAS) unit (OECD, 1993), the Behr KLD-4 unit (Behr Labor-Technik, Düsseldorf-Reisholz) and a UCT-based CAS unit, all fed with a synthetic medium. A description of these systems is given in Schowanek *et al.* (1996) and Rottiers *et al.* (in press) and below in Table 2. The physical/(bio)chemical properties of LAS are listed in Table 3. Measurements of the (parent) removal efficiencies of LAS in the three WWTPs were taken from Rottiers & Decraene (1996). Next to LAS, the fate of hypotheticalum (see Table 1) was also simulated (note that it was assumed that hypotheticalum degrades at the same rate in all three redox zones).

Table 2. Main WWTP design and operation conditions

| | | OECD CAS unit | Behr unit | UCT CAS unit |
|---------------------------------------|--|---------------|-----------------|----------------------|
| volume (anaerobic / anoxic / aerobic) | (L) | - / - / 3.5 | - / 4.2 / 4.5 | 1.5 / 1.5 / 3.0 |
| influent flow | (L/h) | 0.58 | 0.75 | 0.50 |
| loading B _x | (gCOD/gSS.d) | 0.25 | 0.20 | 0.25 |
| SRT | (d) | 10 | 20 | 15 |
| settler recycle ratio | (Q _{recycle} /Q _{influent}) | 0.85 | 2.5 (to anoxic) | 2 (to anoxic) |
| internal recycle ratio | (Q _{recycle} /Q _{influent}) | - | None | 2 (aer. to anoxic) |
| | | | | 2 (anoxic to anaer.) |
| influent LAS concentration | (mg/L) | 1.2 | 2.6 | 3.6 |

Table 3. Properties of the test chemical (LAS) (after Cowan *et al.*, 1993)

| | | | |
|---------------------------------|---|------------------|--|
| K_d (influent & mixed liquor) | (L/kg) | 2000 | solids/liquid partitioning |
| H | (Pa.mol ⁻¹ .m ³) | 10 ⁻⁶ | Henry coefficient |
| $k_{\text{degradation}}$ | (h ⁻¹) | 4* | 1 st order degradation rate |
| | (s/d) | (s+d) | sorbed and/or dissolved phase |
| α_{anoxic} | (-) | 0 | anoxic degradation rate corr. |
| $\alpha_{\text{anaerobic}}$ | (-) | 0 | anaerobic degradation rate corr. |

* obtained by fitting the 6-box model to the OECD CAS standard test measurements

Results and Discussion

Simulated and measured removal efficiencies in the three test systems are shown below in Figure 4. The LAS primary degradation rate (parent compound disappearance) was calibrated, by fitting the 6-box model to the standard OECD CAS test measurements. The calibrated rate of 4 h⁻¹ is slightly higher than the standard value for readily biodegradable chemicals (3 h⁻¹) which is suggested in Struijs *et al.* (1991).

Obviously, the 10-box model resulted in a perfect fit for the single-reactor CAS, as in this case the model is reduced to 6 boxes. For the multiple reactor Behr and UCT units, the predictive power of the 10-box model was superior to the 6-box approach. The 6-box model typically overpredicted LAS effluent concentrations by a factor 1.8. The 10-box model removal prediction was within 0.1% (absolute) of the measurements. Hence, this model allowed to accurately predict LAS removal in 2 nutrient removal plants, using a calibration based on the results of a standard CAS test. Both models predicted a slightly higher removal efficiency in the UCT unit compared to the Behr. However, this was not confirmed by the measurements.

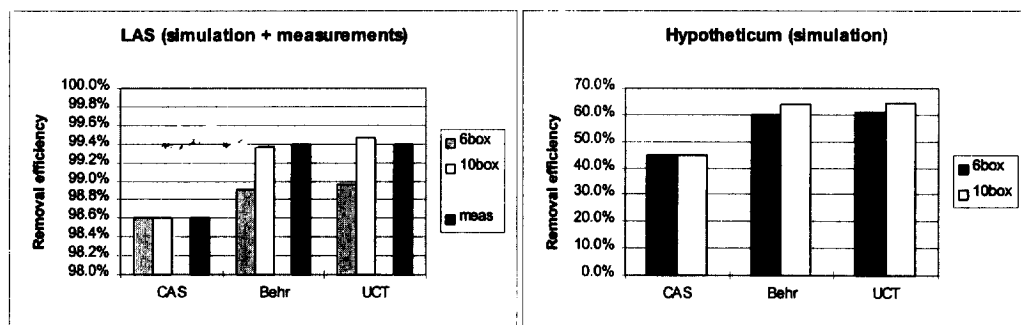


Figure 4. Simulated and measured removal efficiencies in different test systems

For hypotheticum, the 6-box and 10-box model predictions for the CAS unit were identical, as both models are equivalent in this case (see above). For the Behr and UCT units, the 10-box model predicted a higher removal (an absolute difference of more than 3.5%). This trend is similar to what was observed for LAS predictions.

CONCLUSIONS

In this paper it was shown that, by a number of simple modifications, the *SimpleTreat* concept can be adapted to single-sludge nutrient removal WWTPs. A more realistic description of sludge recycling, taking into account the water phase of these recycles and the actual recycling ratios, is proposed. This may improve the fate prediction of highly volatile chemicals.

Two modeling approaches for nutrient removal plants were presented, both based on the UCT design: a 6-box model derived directly from *SimpleTreat*, and a more detailed 10-box model. Simulation results of both models were compared to measured removals for LAS. The degradation rate was calibrated only using available CAS test data, and was subsequently used to predict the fate of LAS in two biological nutrient removal plants. The 10-box model was more accurate than the 6-box model, which underestimated removal. Lower removal predictions by the latter were also found for the default substance hypotheticum.

It is recommended to focus further research on the corroboration of these models for different chemical types. Especially simulation and laboratory measurements of volatile and / or less easily degradable substances would allow to further test the underlying assumptions. This should also give more conclusive evidence on the relative performance of the 6-box versus the 10-box model.

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