Adaptation of *SimpleTreat* to Model Chemical Fate in WWTPs with Biological Nutrient Removal

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Introduction

- **Environmental Risk Assessment:** prediction needed of chemical elimination in WWTPs
- existing **steady-state WWTP fate models** = 'standard' carbon removal plants
- evolution in technology and legislation:
  increasing **importance of biological nutrient removal**

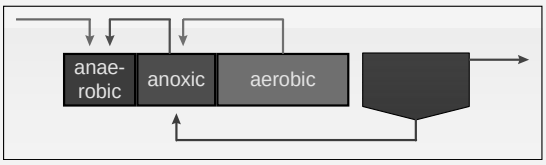
- this work: - **modifications to *SimpleTreat***: - sludge recycling
  - different redox zones in bioreactor
  - **corroboration** for surfactant LAS

Modeling Approach

- state of the art in WWTP fate models: TOXCHEM, AS-TREAT, *SimpleTreat*
- ***SimpleTreat*** model: **used in European Union Risk Assessment**
  → selected for Nutrient Removal modification
- *SimpleTreat* **concept**:
  - standard WWTP = **6 boxes**
    (air, mixed liquor water + solids, settler water + solids, settled sludge)
  - **steady-state mass-balancing**: *SIMPLEBOX* method:
    influx from out of the system + influx from other boxes
    = outflux to other boxes + outflux out of the system + degradation
  - concentrations: solve system of mass balances

Nutrient Removal Plant Configuration

- typical example = **University of Capetown (UCT)** reactor design
  - three activated sludge tanks / zones: **anaerobic, anoxic and aerobic**
  - **internal sludge recycle**: aerobic → anoxic tank and anoxic → anaerobic
  - **settled sludge recycle** to anoxic tank
- other designs: can be simplified to fit this scheme



Sludge Recycling

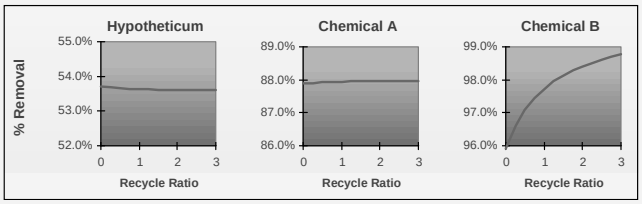
- ***SimpleTreat***: - only solids phase of recycled sludge is considered
  - actual recycle ratios not taken into account

- **Modifications**:
  - **water phase** (+ solutes) of **sludge recycle**:
    → additional advective transport from settler water to activated sludge tank
  - **actual recycle ratio**: flow terms updated

- **Effects of recycle ratio on predicted chemical removal**:(for 3 hypothetical chemicals)

	Hypotheticum	Chemical A	Chemical B
degradation (dissolved)	+	+++	0
sorption	+	+++	+++
volatilization	+	0	+++

  - **simulation results**:
    · non-volatile chemicals: negligible effect
    · **volatile chemical: significant increase in predicted removal**



- **Explanation**: volatile chemicals are also eliminated via settler surface volatilization:
  → **lower dissolved concentration in settler** than in AS tank
  → settler water recycling → dilution in AS-tank dissolved phase
  → desorption from solids due to non-equilibrium
  hence: **larger chemical fraction available for volatilization in AS tank**

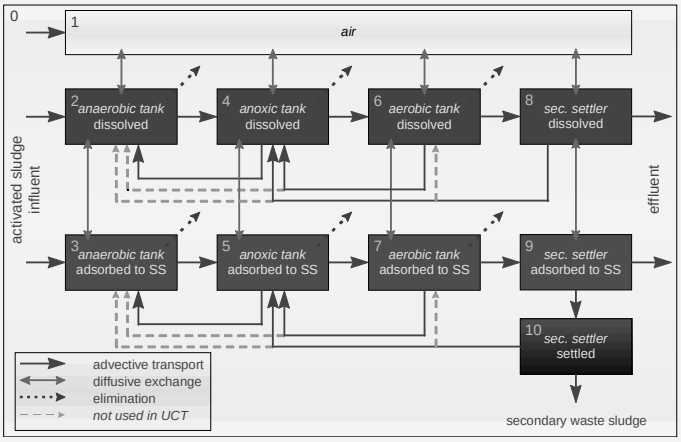
Model Adaptations

6-box model

- very **similar to original** *SimpleTreat* 6-box model
- main modifications:
  - sludge **recycling**
  - correction of **stripping & degradation** (taking into account redox zones)
  - corrected **oxygen requirement**: nitrification / denitrification O_2 balance

10-box model

- direct representation of **UCT process**
  - 3 functionally different AS tanks
    · **biodegradation**: corrected for redox conditons
    · **stripping**: only in the aerated tank
    · surface volatilization in all tanks
  - **internal sludge recycles**



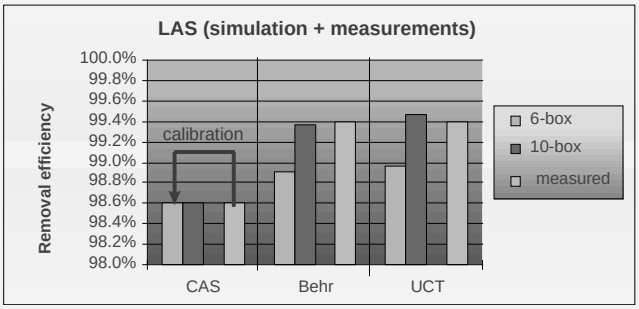
Model Application & Corroboration

Description of Treatment Plants and Chemicals

- fate simulation + laboratory measurements of **Linear Alkylbenzene Sulphonate (LAS)**
- **3 lab-scale activated sludge plants**:
  OECD CAS test (aerobic), Behr KLD-4 (aerobic+anoxic), UCT-based CAS unit

Results and Discussion

- **calibration of LAS degradation rate** (parent degradation only):
  fitting 6-box model to standard OECD CAS test results → **k = 4 h^{-1}**
  (cf. 'default' for readily biodegradable chemicals = 3 h^{-1})
- 6-box versus 10-box model results:
  - perfect fit for CAS (model reduced to 6-box = calibration case !)
  - multiple reactor Behr + UCT units:
    10-box model had higher predictive power than 6-box
- 10-box model removal prediction within 0.1% (absolute) of measured removal
  → **10-box model** allowed to **accurately predict LAS removal** in 2 BNR plants,
  using a calibration **based on the results of a standard OECD CAS test**
- 6-box model slightly underestimated removal efficiencies



Conclusions

- by a number of **simple modifications**, the ***SimpleTreat*** concept could be adapted to **single-sludge nutrient removal WWTPs**
- more realistic description of **sludge recycling** is proposed
  → may improve fate prediction of highly **volatile chemicals**
- 2 approaches (based on UCT design): **6-box and 10-box model were presented**
- **10-box model** allowed to **accurately predict LAS removal** in 2 BNR plants, using a calibration based only on the results of a standard OECD CAS test
- recommendation: **focus further research on corroboration** for different chemicals

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