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MODELING – AN IMPORTANT WATER MANAGEMENT TOOL

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1. Introduction
2. Results
3. Summary
1. Introduction
Water Research at TU Berlin

- Centre for Water in Urban Areas since 2000 (FSP-WIB)
- Cooperation contracts many external partners: Berlin Centre of Competence for Water, BWB, Bayer etc.
- 22 chairs merging their water knowledge over 5 faculties

- Four core fields of activity

Innovation  Analytics  Economy  International
MAIN OBJECTIVES

Development a model-based integrated management tool to:

- predict the economical and calculate the ecological effects (e.g. impact on water bodies) of water recycling and the related technologies
- optimize water treatment technologies, processes and sites
- demonstrate the potential for freshwater savings, the recovery of heat and valuables
METHODOLOGY

**Integrated Urban Water Cycle**

- **Process Level**
- **Process Unit Level**
- **Fundamentals**

**Fundamentals**
- Fundamentals of System and Process Engineering
- Environmental Process Engineering
- Wastewater Process Engineering
MODELS DEVELOPED

PVC production process

• Polymerization reactor performance model
• Wet cooling tower performance model
• General mass and energy balance model

Wastewater treatment process

• Heat exchanger model
• MBR ASM, ion removal, energy consumption (aeration and pumping) models
• RO ion removal, energy consumption models
• Ultrafiltration/Nanofiltration models

Other models

• Electrodialysis model (Master thesis with TNO)
• Membrane distillation model
• Activated carbon adsorption model
2. Results
INOVYN CASE

Concentrated Flow

Excess Sludge

Cooling Tower

Cooling Water

Recycled Wastewater

RO

MBR

Heat Exchange 2

Heat Exchange 1

Filter

Wastewater

Recycled Wastewater
Steady state calibration:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Measured value</th>
<th>Default ASM1 values</th>
<th>Default mbr_ASM1HSG values</th>
<th>Calibrated ASM 1 values</th>
</tr>
</thead>
<tbody>
<tr>
<td>NH4+-N</td>
<td>g m⁻³</td>
<td>1.1</td>
<td>0.14</td>
<td>0.25</td>
<td>0.64</td>
</tr>
<tr>
<td>NO3-N</td>
<td>g m⁻³</td>
<td>12.1</td>
<td>6.2</td>
<td>6.5</td>
<td>12.0</td>
</tr>
<tr>
<td>MLSS</td>
<td>g m⁻³</td>
<td>11254</td>
<td>12970</td>
<td>11720</td>
<td>11580</td>
</tr>
</tbody>
</table>

Avg. Values over 100 days (pilot and model)
Dynamic state calibration:

The graph shows the comparison of simulated and measured concentrations of NH4-N and NO3-N over time. The concentrations are measured in mg L^-1. The simulated values are represented by solid lines, while the measured values are represented by dotted lines. The x-axis represents time in days, ranging from 0 to 100 days. The y-axis represents the concentration in mg L^-1, ranging from 0 to 40 for NH4-N and 0 to 16,000 for NO3-N.

The graph indicates that there is a good alignment between the simulated and measured concentrations, suggesting that the model is accurately representing the dynamic state of the system.
### SCENARIOS FOR LCA

#### Parameter

<table>
<thead>
<tr>
<th>Different recovery scenarios</th>
</tr>
</thead>
<tbody>
<tr>
<td>25%</td>
</tr>
<tr>
<td>50%</td>
</tr>
<tr>
<td>75%</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Recycled water flow (m³/d)</th>
</tr>
</thead>
<tbody>
<tr>
<td>600</td>
</tr>
<tr>
<td>1200</td>
</tr>
<tr>
<td>1800</td>
</tr>
</tbody>
</table>

#### MBR parameters

<table>
<thead>
<tr>
<th>Chemicals consumes (kg/d)</th>
<th>K2HPO4</th>
<th>Antifoam</th>
<th>NaOH</th>
<th>C6H8O7</th>
<th>NaClO</th>
<th>HCl</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy consumption (kWh/m³ water)</td>
<td>0.74</td>
<td>0.74</td>
<td>0.74</td>
<td>0.74</td>
<td>0.74</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Chemicals consumes (kg/d)</th>
<th>Antiscalant</th>
<th>Biocide</th>
<th>Acid cleaning</th>
<th>Alkaline cleaning</th>
<th>Surfactant</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy consumption (kWh/m³ water)</td>
<td>0.81</td>
<td>0.96</td>
<td>1.27</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

#### RO parameters

<table>
<thead>
<tr>
<th>Chemicals consumes (kg/d)</th>
<th>Antiscalant</th>
<th>Biocide</th>
<th>Acid cleaning</th>
<th>Alkaline cleaning</th>
<th>Surfactant</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy consumption (kWh/m³ water)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>


GROUNDWATER AND COSTS SAVED

<table>
<thead>
<tr>
<th>Wastewater recycling ratio</th>
<th>Recycled wastewater (m³/d)</th>
<th>Fresh groundwater required (m³/d)</th>
<th>Costs of groundwater (Euros/d)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0%</td>
<td>3,418</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>10%</td>
<td>2,809</td>
<td>1,549</td>
<td>2,890</td>
</tr>
<tr>
<td>20%</td>
<td>2,389</td>
<td>1,129</td>
<td>2,389</td>
</tr>
<tr>
<td>30%</td>
<td>1,969</td>
<td>709</td>
<td>1,969</td>
</tr>
<tr>
<td>40%</td>
<td>1,549</td>
<td>389</td>
<td>1,549</td>
</tr>
<tr>
<td>50%</td>
<td>1,129</td>
<td>0</td>
<td>1,129</td>
</tr>
<tr>
<td>60%</td>
<td>709</td>
<td>0</td>
<td>709</td>
</tr>
<tr>
<td>70%</td>
<td>289</td>
<td>0</td>
<td>289</td>
</tr>
<tr>
<td>80%</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
HEAT ENERGY

Heat required in reactor (kWh/m³) vs. Recycled wastewater temperature (°C) for different Wastewater recycling ratios:

- 0% recycling: 65.3°C
- 10% recycling: 55.9°C
- 20% recycling: 49.9°C
- 30% recycling: 45.1°C
- 40% recycling: 41.2°C
- 50% recycling: 37.8°C
- 60% recycling: 34.7°C
- 70% recycling: 31.9°C
- 80% recycling: 29.3°C
Recycled wastewater quality

NH₄⁺, K, Mg, As, Ca concentrations (mg/L) and COD, Cl concentrations (mg/L) and conductivity (μS/cm) vs. wastewater recycling ratio.
DISCHARGED WASTEWATER QUALITY

The quality meets the discharge limits
3. Summary
MAIN OUTCOMES

✓ Integrated model to predict:
  ✓ Water consumption
  ✓ Water quality
  ✓ Energy usage
  ✓ Scenarios
  ✓ Environmental impact (together with LCA)

✓ Transfer to other sites ➔ can be used to visualize flows for planned and existing sites

✓ Training of employees

✓ Process models:
  ✓ Combining them to simulate treatment trains
  ✓ Predict effluent qualities
  ✓ Scenario analysis
Dear all,

After the presentation of your work at Inovyn some weeks ago, we saw the big potential of this tool.

Hence, we are trying to hire a bachelor student during this summer period to run some scenarios and validate the model for different operation modes.

Our aim is to use this model to develop water strategies for future working conditions in our site which can significantly change in few years.

Thus, we would need a Simba license extension until September 2016 to be able to perform these simulations.

Do you think you can get this license extension for us?

We keep in contact on Wednesday during final conference.

Best Regards,

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David Prieto de la Parte
Chemical Engineer
Thank you for your attention!