Validation of a multi-phase Plant-Wide Model for the description of the aeration system in a WWTP

Guaranteeing energetic, environmental and economic sustainability

Mathematical modelling: useful tool for optimum solutions

Biological processes are still important but also Chemical and physico-chemical processes

Update of conventional mathematical models considering these processes
Modeling of mass transfer between gas and aqueous phases in WW systems

- Conventional models:
  - Gas-liquid transfer focused on oxygen dissolution
  - Model based empirical parameters

\[ OTR = k_L a \cdot (DO_{sat} - DO) \cdot V \]

- Current models:
  - Much more interest on the size, contact area, composition, temperature, pressure of gaseous phases
    - Oxygen transfer efficiency OTE prediction
      \[ OTE = \frac{Q_{air, in} \cdot Y_{O_2, in} - Q_{air, out} \cdot Y_{O_2, out}}{Q_{air, in} \cdot Y_{O_2, in}} \times 100 \]
    - Water buffer capacity description
    - Study of technologies with different gaseous phases (ATAD, pure O₂)
MODELLING OF MASS TRANSFER BETWEEN GAS AND AQUEOUS PHASES IN WW SYSTEMS

- ASM models (Henze et al., 2000)
- ADM1 model (Batstonte et al., 2002)

Only biological reaction are represented by the product $E \cdot \rho$

G-L mass transfers are considered without systematic representation

Example:

$$\frac{dC}{dt} = \frac{Q}{V} \left( C_{in} - C \right) + E \cdot \rho$$

$$\frac{dDO}{dt} = \left[ \frac{dC}{dt} \right]_{DO} + k_L a \cdot (DO_{sat} - DO)$$
1. To develop a systematic methodology for the gas/liquid mass transfer in wastewater/sludge systems
   • Coupled to biochemical and chemical models
   • Based on physical parameters

2. From a case study in a real WWTP
   • To develop, calibrate and validate a mathematical model developed according to this methodology
     – Describing the oxygen transfer efficiency in aerated reactors
- **Systematic and flexible procedure** to construct Unit-process models

- **Mass and charge continuity in the transformations**
  Components definition with elemental mass and charge characterization

- **Mass transport**: Systems where components in liquid, gaseous or solid phase coexist

- Include biochemical + chemical + physico-chemical transformations

- Guarantees heat conservation in all transformation and in every unit-processes

- Incorporates operational costs
**Example: Biological Aerated Closed Reactor**

- **Composition off-gas phase ≠ Composition hold up phase**
- **Temperature off-gas phase ≠ Temperature hold up phase**
- **Contact surface off-gas-water phase ≠ Contact surface hold up-water phase**
**Description of the L-G Mass Transfer**

\[
\begin{align*}
\frac{dM}{dt} &= I/O_{\text{terms}} + \sum E_{1,1} \cdot \rho^*_{1,1} + \sum E_{1,2} \cdot \rho^*_{1,2} + \sum E_{1,3} \cdot \rho^*_{1,3} \\
\frac{dM}{dt} &= I/O_{\text{terms}} + \sum E_{2,1} \cdot \rho^*_{2,1} \\
\frac{dM}{dt} &= I/O_{\text{terms}} + \sum E_{3,1} \cdot \rho^*_{3,1}
\end{align*}
\]

**Units:** mass

**Internal Transformations**
- 1. Aerobic consumption SSU
- 2. CO2 equilibrium
- 3. Aerobic decay XH

**Mass Transport**
- 1. Mass transport with liquid phase
- 2. Mass transport with gaseous phases

**Mass Exchange with Liquid Phase**
- Mass exchange with liquid phase
- Mass exchange with gaseous phases

**Units:** mass/time
**DESCRIPTION OF THE L-G MASS TRANSFER**

**LIQUID-GAS TRANSFER KINETIC EXPRESSIONS:**

\[ KL,i = f(D_i, T) \]

\[ \alpha \triangleq \text{difference between clean and process water} \]

\[ \rho_{w,\text{off}} = \alpha \cdot KL,i \cdot A_{\text{off}} \cdot \left( K_{H,i} \cdot P_{\text{off},i} - C_i \right) \]

\[ \rho_{w,\text{ghu}} = \alpha \cdot KL,i \cdot A_{\text{ghu}} \cdot \left( K_{H,i} \cdot P_{\text{ghu},i} - C_i \right) \]

\[ P_{\text{off},i} \rightarrow \text{IG law} \]

\[ P_{\text{ghu}} = P_{\text{off}} + \frac{1}{2} \cdot \frac{V_L}{A_{\text{off}}} \cdot \frac{1}{10.33} \]

\[ A_{\text{ghu}} = \frac{6V_{\text{ghu}}}{d_b/F} \]

\( d_b \rightarrow \text{bubble diameter} \)

\( F \rightarrow \text{incaesment in the bubble diameter by the fouling of the diffusers} \)
Case Study

Estimation of the Oxygen Transfer Efficiency (OTE) in Galindo WWTP and its Effects on Biological Activity, Energetic Requirements and Costs

- Galindo-Bilbao WWTP:
  - 1.5 millions population equivalent
  - 6 parallel lines for COD and N removal
  - R-DN configuration
  - Height of the reactors: 9 m
**CATEGORIES**

- **COD removal** (Aer., Anox)
- **N removal**
- **Chemical equilibria**
- **Liquid gas transfer**

**UNIT PROCESS MODELS**

- Completely Stirred Closed Tank Reactor
- Completely Stirred Open Tank Reactor
- Intermittently Open Tank Reactor
- Buffer Tank
- Membrane bioreactor
- Primary Clarifier
- Secondary Clarifier
- Layered Settler
- Thickener / Dewatering
- Biofilm reactor
- Heat exchanger
- Precipitator
- Cogeneration unit
- Incineration unit

**ACTUATOR MODELS**

- Blowers
- Hydraulic pump
- Pump ejector
- Agitation engine
- Heating equipment
MODEL CONSTRUCTION

\[
OTE = \frac{\text{Q}_{\text{air, in}} \cdot Y_{\text{O}_2, \text{in}} - \text{Q}_{\text{air, out}} \cdot Y_{\text{O}_2, \text{out}}}{\text{Q}_{\text{air, in}} \cdot Y_{\text{O}_2, \text{in}}} \cdot 100
\]
Model Calibration and Validation

Measurement of OTE
- 8 experimental campaigns (1 week per each)
- According to ASCE protocol
  - 3% of the surface of the aerated tank covered
  - Supplied air flowrate kept constant

Measurements
- \( \text{O}_2 \) and \( \text{CO}_2 \) composition of extracted gas
- Extracted off-gas flow rate
- Extracted gas temperature
- Dissolved oxygen
- Water temperature
- Environmental conditions (atmospheric pressure, temperature and relative humidity)
### Model Calibration and Validation

#### Measured OTE (Average of Each Reactor)

<table>
<thead>
<tr>
<th></th>
<th>R1</th>
<th>R2</th>
<th>O1</th>
<th>O2</th>
<th>O3</th>
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<td>22.0</td>
<td>24.5</td>
<td>22.1</td>
</tr>
</tbody>
</table>
Model Calibration and Validation

- Steady-state simulations for the 8 experimental campaigns

- Assumed parameters:
  - $\alpha = 0.85$ (Gillot & Héduit, 2008)
  - $K_{L,O2} = 0.074$ (Vogelaar et al., 2000)
  - $K_{L,CO2} = f(K_{L,O2})$
  - $K_{L,N2} = f(K_{L,O2})$

- Calibration of $\text{db}/F$
  - $\text{db}/F = 2.23$
    - $\text{db} = 1.8\text{ mm}$
    - $F = 0.8$ (Trillo, 2004)

$\alpha F = 0.68$
Model Validation

- Dynamic simulation for the year 2013 was run

Air flow rate (Controlled variable by N-NH4 set-point)

- The model predicts properly the OTE in Galindo WWTP
- $\alpha F = 0.68$
**Kla and Gas Phases Composition**

### Kla in All Reactors

<table>
<thead>
<tr>
<th></th>
<th>Anox</th>
<th>Aer 1</th>
<th>Aer 2</th>
<th>Aer3</th>
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<td>20</td>
<td>104</td>
<td>11</td>
</tr>
</tbody>
</table>

### Gas Composition in All Gaseous Phases

- **Atmosphere**
  - $O_2$: 21%
  - $CO_2$: 79%
  - $N_2$: 0%
  - $NH_3$: 0%

- **GAS HOLD-UP AEROBIC REACTOR**
  - $O_2$: 14%
  - $CO_2$: 84%
  - $N_2$: 2%
  - $NH_3$: 0%

- **GAS HOLD-UP ANOXIC REACTOR**
  - $O_2$: 10%
  - $CO_2$: 85%
  - $N_2$: 5%
  - $NH_3$: 0%

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EFFECT OF BUBBLE SIZE AND SUBMERGENCE OF DIFFUSERS ON OTE

OTE increases
- Increase of the bubbles residence time

OTES decreases
- Reduction in the contact area between liquid and gaseous phase
- Increase in the ascensional velocity of the bubbles (decrease of the residence time)
Motivation & Objectives

Fundamentals of Extended PWM methodology

CEIT Plant-Wide Modelling library

Case Study

Conclusions
Conclusions

• The methodology proposed allows the construction of a physico-chemical model able to describe the different gasesous phases existing in a biological reactor
  • The detailed description of these gasesous phases implies some important advantages:
    • OTE is calculated by the model without extra information from the suppliers
    • Water chemistry is calculated correctly
    • Other novel technologies (ATAD, pure oxygen) can be modelled

• From the case study
  • The model was able to describe the oxygen transfer efficiency in Galindo WWTP
  • The model described the different gasesous phases in aerated and anoxic reactors according to the environmental conditions of each reactor
  • The model allows the analysis by simulation of the effect of physical paramenters on the OTE
Validation of a multi-phase Plant-Wide Model for the description of the aeration system in a WWTP


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