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

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Summary of key findings
This paper introduces a new mathematical model built under a new physico-chemical modelling methodology to describe the liquid-gas transfer in a WWTP. The mathematical model constructed is able to reproduce biological COD and nitrogen removal, liquid-gas transfer of O₂, N₂ and CO₂, chemical reactions for pH calculation and the effect of each of them on the other. The capability of the model has been checked by comparing simulated and experimental results in a full-scale WWTP, specifically focused on assessing the aeration system efficiency. Finally, an exploration by simulation has been undertaken to study the effect of design and operation parameters such as reactor height or aeration with pure oxygen in liquid-gas transfer efficiency.

Background and relevance
Nowadays, chemical and liquid-gas transfer processes are becoming very prominent in technologies and ways of design and operation of WWTP due to a generalized concern about climate change and scarcity of natural resources. Specifically, liquid-gas transfer is crucial to study several aspects, such as: the efficiency of the aeration system in a WWTP for the reduction of energy consumption; the greenhouse gases emissions or the efficiency of the dissolved air flotation technology, which strongly depends on the bubble formation mechanism. In this context, the main challenge of the scientific community is to obtain modelling methods for describing chemical and physico-chemical processes. In this sense, several works have been developed for the description of the liquid-gas transfer processes to particularly describe the oxygen transfer in aerated systems with a different level of detail (Gillot et al., 2005; Beltrán et al., 2013). However, these mathematical models are based on empirical relationships and their predictive capacity for different conditions or gases other than O₂ is limited.

Considering the limitations of the existing models and the new requirements for the models, the objective of this paper is to construct and validate a mechanistic model able to represent the biochemical, chemical and liquid-gas transfer reactions in a WWTP based on physical parameters, rather than empirical parameters. The mathematical model is calibrated and validated using experimental data collected in Galindo-Bilbao WWTP. Finally, an exploration by simulation is carried out to assess the effect of reactor height and aeration with pure oxygen on the transfer efficiency.

Results
Construction of the mathematical model
The model has been constructed using the Physico-chemical Plant-Wide Modelling (PC-PWM) methodology proposed by Lizarralde et al. (2015) which offers a systematic way to jointly consider biochemical, chemical and physico-chemical processes. This methodology requires two steps: (i) the definition of the model components and transformations and (ii) mass transport definition for a multi-phase model of WWTP. The main characteristics of the model are described below.

The model components and transformations are selected to describe the dynamic COD and nitrogen removal and reproduce the liquid gas transfer of O₂, N₂ and CO₂ that allows the estimation of oxygen transfer efficiency. The details of the model for the definition of the model components and transformations can be found in Lizarralde et al. (2015).

For the mass transport definition three steps need to be followed. First, the phases that are present in the system need to be defined. The unit processes required are open reactor with and without aeration for which three phases are considered. One of them represents the aqueous phase, another represents the open atmosphere on top and the last one represents the gas hold-up phase describing in the aerobic reactor the air flow rate introduced or in the anoxic reactor the gaseous phase formed due to biological activity. In both cases the composition of the gas hold-up phase depends on biological activity and pH. Second, the reactions inside phases and interactions among them are specified. All transformations
take place in the aqueous phase and there is interaction between the phases. Finally, as each phase included in the model is considered as a completely stirred reactor mass balances are applied to each phase present in the model.

\[
\rho_{\text{v, off}} = \frac{k_{L1}}{A \left( \frac{P_{\text{off}} - C_i}{P_{\text{in}}} \right)} \\
\rho_{\text{v, gas, b}} = \frac{k_{L2}}{A \left( \frac{P_{\text{gas, b}} - C_i}{P_{\text{in}}} \right)} \\
a = \frac{6 V_{\text{gas, b}}}{d_b} \\
V_{\text{gas, b}} = \frac{n_{\text{gas, b}}}{z \cdot R \cdot T} \\
P_{\text{gas, b}} = \frac{P_{\text{in}} \cdot \frac{V_{\text{gas}}}{2 \cdot A \cdot 10.33}}{n_{\text{gas, b}}} \\
V_{\text{gas}}: \text{total volume of the bubbles} \\
n_{\text{gas, b}}: \text{number of moles of gas contained in the gas hold-up phase}
\]

\(\text{OTE} = \frac{Q_{\text{in, air}} \cdot Y_{O_2, \text{in}} - Q_{\text{out, air}} \cdot Y_{O_2, \text{out}}}{Q_{\text{in, air}} \cdot Y_{O_2, \text{in}}} \cdot 100\)

Where:
- \(Q_{\text{in, air}}\): air flow rate in
- \(Q_{\text{out, air}}\): air flow rate out
- \(Y_{O_2, \text{in}}\): molar fraction of oxygen in the inlet
- \(Y_{O_2, \text{out}}\): molar fraction of oxygen in the gas hold-up

Specifically, the bubble size is a key parameter in the calculation of the OTE, due to its effect over two aspects: (i) the smaller the bubble the lower the up-flow velocity, thus the higher the contact time and higher (ii) it determines the specific surface available for liquid-gas transfer.

**Full-scale validation of the oxygen transfer mathematical model**

The objective of this validation is to check the capability of the model to reproduce the real performance of the aeration system in Galindo-Bilbao WWTP. The biological treatment in the water line of Galindo WWTP treats 4m³/s and contains six equal lines for organic matter and nitrogen removal (Beltrán et al., 2014). A series of experimental campaigns were carried out in Galindo-Bilbao WWTP to study the efficiency of the diffusers based on the methodology presented in the ASCE-18-96 (1997) report. In total, eight experimental campaigns where carried out to test the six lines under different operating configurations during 9 months. The results of the experimental campaigns are gathered in Beltrán et al. (2014). The parameter adjusting procedure was based on the steady state conditions during the first experimental campaign. During the simulations the diameter of the bubbles was adjusted in order to match, as far as possible the OTE measured experimentally. In order to achieve the best adjustment the bubble diameter is 2 mm. For the validation, the value adjusted for the bubble diameter for the first experimental campaign was kept constant and simulations for the rest of experimental campaigns were run. Applying these conditions, the fit between experimental and simulated results (Figure 2) is relatively good.

**Table 1 Composition of the gas hold-up simulated and experimentally measured**

<table>
<thead>
<tr>
<th></th>
<th>Anox</th>
<th>Reactor 1</th>
<th>Reactor 2</th>
<th>Reactor 3</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Sim</td>
<td>Exp</td>
<td>Sim</td>
<td>Exp</td>
</tr>
<tr>
<td>%O₂</td>
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<td>15.5</td>
<td>16.9</td>
<td>17.3</td>
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<tr>
<td>%N₂</td>
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<td>82.7</td>
<td>81</td>
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</tr>
<tr>
<td>%CO₂</td>
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<td>1.8</td>
<td>2.1</td>
<td>1.8</td>
</tr>
<tr>
<td>GluH₂O₂</td>
<td>24</td>
<td>121</td>
<td>13</td>
<td>102</td>
</tr>
<tr>
<td>GluH₂</td>
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<td>20</td>
<td>106</td>
<td>11</td>
</tr>
<tr>
<td>GluH₂O</td>
<td>0.7</td>
<td>20</td>
<td>104</td>
<td>11</td>
</tr>
</tbody>
</table>

**Figure 2 Comparison of experimental and simulated OTE in the aerated reactors**

Figure 2 shows the comparison of the simulated OTE versus experimentally measured OTE under the same conditions in the aerated reactors. It is observed that the simulated data follow the trend of experimental data with the 5% of error. Additionally, the model is able to predict the measured composition of the gas hold-up phase in the aerated reactors (Table 1). Finally, separating the traditionally used \(k_{L1} a\) value into a \(k_L\) parameter and a variable representing the specific interphase area...
enables reproducing the transfer of the oxygen and the rest of the gases independently. For example, in the reactors which are not aerated the contact area of the oxygen (a) is null. If the traditional approach would be used the $k_{L,a}$ of other gases would need calibration, whereas with this new approach, $k_{L}$ of all gases is calculated through the $k_{L}$ of the oxygen but the area is calculated independently (Table 1).

This enables a right description of gas stripping, particularly of CO$_2$ which allows predicting pH correctly since the accumulation of the total dissolved carbonate system is avoided.

Exploration by simulation of the effect of reactor height and aeration with pure oxygen on air flow rate

In the exploration by simulation two effects have been analysed. First the combined effect of the bubble diameter and reactor height has been analysed and second the alternative of using pure oxygen or combining pure oxygen and air for aeration has been studied.

The effect of the diffusers submergence and the bubble diameter on the OTE has been analysed (Figure 3, Left) by running 100 simulations. It can be seen that the higher the submergence the higher the transfer efficiency due to two mechanisms: on the one hand, the higher the submergence of the diffusers the higher the pressure exerted by the column of water increasing the solubility of oxygen in water. And on the other hand, the higher the column of water above the diffuser, the higher the contact time between the gaseous and liquid phase. It can be seen that the transfer efficiency is lower when bigger bubbles are formed due to clogging. This effect is strengthened when working in short reactors.

The alternative of using pure oxygen for aeration can be also analysed (Figure 3, Right). It has been observed that the volumetric flow requirements are up to 70% lower as expected. Even though the volumetric flow requirement is lower and consequently pumping costs may be reduced, the high costs of pure oxygen makes this alternative non appropriate for urban WWTP. This is the reason why the alternative of using pure oxygen in combination with air when the influent load is high has been analysed. A constant air flow rate has been set during the whole year and pure oxygen is injected when oxygen demand is higher than the given by air. This alternative lowers the volumetric flow in 40% (Figure 3, Right). This exploration shows the potential of the model to analyse the possibility of using different gases for aeration.

**Figure 3 (Left) Effect of height on oxygen transfer efficiency; (Right) Effect of aerating with pure oxygen**

**Discussion**

A new mathematical model developed under the Physico-Chemical Plant-Wide modelling (PC-PWM) has been built. Its ability to reproduce the aeration system of a real WWTP has been tested experimentally. The model performance and capacity have been checked with data taken from a real WWTP. The simulations have shown the interesting results and practical benefits of using this kind of mathematical models for process operation analysis.

**References**


