Prediction of the gas–liquid volumetric mass transfer coefficients in surface-aeration and gas-inducing reactors using neural networks

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Received 6 May 2002; received in revised form 30 October 2002; accepted 30 October 2002

Abstract

Almost all available literature correlations to predict the volumetric gas–liquid mass transfer coefficient, \( k_{L,a} \) in agitated reactors are systems- or operating conditions-dependent. In this study, two back-propagation neural networks (BPNNs), one dimensional and one dimensionless were developed to correlate \( k_{L,a} \) for numerous gas–liquid systems in both surface-aeration reactors (SAR) and gas-inducing reactors (GIR) operating under wide ranges of industrial conditions. A total of 4435 experimental data points obtained from more than 10 publications for 50 gas–liquid systems were used to train, validate the dimensional and dimensionless BPNNs, which were able to correlate all \( k_{L,a} \) values with \( R^2 \) of 90.5 and 88.6%, respectively. The dimensional BPNN was used to predict the effect of various operating parameters on \( k_{L,a} \) in a number of important industrial processes. The predictions showed that increasing liquid viscosity decreased \( k_{L,a} \) values in the SAR, while \( k_{L,a} \) values in the GIR increased and then decreased with increasing liquid viscosity, following the gas holdup behavior. Increasing liquid density decreased \( k_{L,a} \) in both reactor types. Increasing liquid surface tension increased \( k_{L,a} \) values in the SAR, whereas in the GIR, \( k_{L,a} \) decreased due to the increase of bubble size. Increasing gas diffusivity or gas partial pressure or mixing speed, increased \( k_{L,a} \) in both reactor types. \( k_{L,a} \) values in the GIR were always higher than those in the SAR and increasing \( D_{imp}/D_T \) and \( H_L/H_g \) increased \( k_{L,a} \) in both reactor types.

Keywords: Back-propagation neural network; Gas–liquid systems; Gas-inducing reactors; Surface-aeration reactors; Volumetric gas-liquid mass transfer coefficient

1. Introduction

The design, scale-up and optimization of industrial processes conducted in multiphase agitated reactors require, among others, precise knowledge of the hydrodynamics, mass and heat transfer parameters and reaction kinetics. Literature data available indicate that the gas–liquid mass transfer is generally the rate-limiting step in many industrial processes [1] and hence the focus of this paper is on the assessment of the volumetric gas–liquid mass transfer coefficient, \( k_{L,a} \), in agitated reactors. Tables 1 and 2 present available literature correlations for \( k_{L,a} \) in surface-aeration reactors (SAR) and gas-inducing reactors (GIR), respectively. From these tables it appears that these correlations were proposed to predict \( k_{L,a} \) values for a specific gas–liquid system under ambient conditions or high pressures and temperatures as a function of dimensionless numbers [3–6,8,15–23], specific power input [2,3,7,11–13,24] or non-linear statistical correlations [9,10]. Although supposedly independent of the gas–liquid system, \( k_{L,a} \) values predicted using the dimensionless correlations often provide large deviations when compared with experimental data [25–27]. Similarly, \( k_{L,a} \) predicted using the specific power input correlations frequently deviates from the actual experimental values obtained under typical industrial conditions, since these correlations do not directly account for the effects of pressure and/or temperature on \( k_{L,a} \). The statistical correlations, on the other hand, are claimed to predict \( k_{L,a} \) with confidence levels greater than 97.5% [9,10,28,29], but they are specific to the gas–liquid system and reactor employed. Thus, there is a great need for developing \( k_{L,a} \) correla-
Recently, artificial neural networks (ANNs) have been employed in different industrial applications in order to describe, control or model complex chemical processes, as shown in Tables 3 and 4. Iliuta et al. [35] used neural networks to correlate $a$ and $k_{L}a$ in trickle-bed reactors over wide ranges of industrial operating conditions. Yang et al. [25] developed a neural network to correlate $k_{L}a$ in gas sparging reactors (GSR), operating under atmospheric conditions, however, their study was limited to oxygen transfer into a Newtonian coalescing liquid.

The purpose of this study is to develop a more general and system-independent correlation based on back-propagation neural networks (BPNN), which accounts for the various observed trends of $k_{L}a$ in the literature for SAR and GIR. The methodology used to develop and validate the neural networks was described and one dimensionless and another dimensional ANN correlations were developed. The dimensional neural network
<table>
<thead>
<tr>
<th>Authors</th>
<th>Induction type</th>
<th>Gas</th>
<th>Liquid</th>
<th>Operating conditions</th>
<th>Correlations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Joshi and Sharma [11]</td>
<td>Hollow shaft + Hollow impeller</td>
<td>CO₂</td>
<td>Na₂CO₃ + NaHCO₃</td>
<td>0.41 &lt; Dr &lt; 1.0, 0.35 &lt; Dimp/Dr &lt; 0.75, H₂/Dr &lt; 0.5, Dimp/10 &lt; Himp &lt; Dimp/3, 3 &lt; N' &lt; 11.7 Hz, 0.0003 &lt; U₇G &lt; 0.032 m·s⁻¹, 1 &lt; P*/V₇ &lt; 15 kW/m³, 0.04 &lt; kₗa &lt; 0.3 s⁻¹</td>
<td>U₇G &lt; 0.005: kₗa = 6.8 × 10⁻¹⁴(P*/V₇)⁰.⁵⁵U₇G⁰.⁵¹⁵; U₇G &gt; 0.005: kₗa = 3.26 × 10⁻¹⁵(P*/V₇)⁰.⁵⁵U₇G²⁵³</td>
</tr>
<tr>
<td>Kara [12]</td>
<td>Hollow shaft + Rushton turbine</td>
<td>H₂</td>
<td>Tetraline SRCI</td>
<td>70—135 bar, 606—684 K, 50—400 rpm, P*/V₇ &lt; 119 W/m³</td>
<td>kₗa = (3.43 ± 1.13) × 10⁻⁴(P*/V₇)⁰.⁵⁵</td>
</tr>
<tr>
<td>Sawant et al. [13]</td>
<td>Denver type impeller</td>
<td>Air</td>
<td>Water + sodium sulfate</td>
<td>5 &lt; N &lt; 36 rev/s, 0.5 &lt; H'/Dimp &lt; 1.5</td>
<td>kₗa = 0.0195 × (P*/V₇)⁰.⁵⁵</td>
</tr>
<tr>
<td>Karandikar et al. [14]</td>
<td>Hollow shaft + Rushton turbine</td>
<td>CO</td>
<td>F-T wax</td>
<td>7—45 bar, 423—498 K, 700—1000 rpm</td>
<td>CO and H₂: kₗa = 0.1607(N/1000)³ · 4²; exp(0.108 × P) — 0.046</td>
</tr>
<tr>
<td>Chang et al. [15]</td>
<td>Hollow shaft + Rushton turbine</td>
<td>N₂</td>
<td>n-hexane</td>
<td>177 &lt; Eu &lt; 2232, 1913 &lt; We &lt; 7239, 8.6 &lt; Sc &lt; 28.5, 146000 &lt; Re &lt; 290000</td>
<td>Sh = 6.67 × 10³³⁸Re⁻²⁶</td>
</tr>
<tr>
<td>Chang and Morsi [16]</td>
<td>Hollow shaft + Rushton turbine</td>
<td>N₂</td>
<td>Water, n-hexane</td>
<td>560 &lt; Eu &lt; 10960, 760 &lt; We &lt; 7410, 14 &lt; Sc &lt; 128, 102400 &lt; Re &lt; 282600</td>
<td>Sh = 2.39 × 10⁻²⁸Re⁻⁴⁸</td>
</tr>
<tr>
<td>Chang and Morsi [17]</td>
<td>Hollow shaft + Rushton turbine</td>
<td>N₂</td>
<td>n-decane</td>
<td>1582 &lt; We &lt; 6528, 63433 &lt; Re &lt; 216626, 1.15 &lt; Fr &lt; 2.59</td>
<td>Sh = 2.95 × 10¹⁴Re⁻¹⁴¹Fr⁻⁴³⁷We⁻¹³²⁶</td>
</tr>
<tr>
<td>Dietrich et al. [18]</td>
<td>Hollow shaft + Rushton turbine</td>
<td>H₂</td>
<td>Water, ethanol, hydrogenation mixt. of adiponitril</td>
<td>Vₑ = 500 ml, 0.25 &lt; V₇ &lt; 0.38 dm³</td>
<td>H/R = 1: Sh = 3 × 10⁻¹⁴Re⁻¹⁴⁵</td>
</tr>
<tr>
<td>Hichri et al. [19]</td>
<td>Hollow shaft + Turbine</td>
<td>H₂</td>
<td>2-propanol o-cresol</td>
<td>10⁴ &lt; Sh &lt; 5 × 10⁵, 7 × 10³ &lt; Re &lt; 13 × 10⁴, 500 &lt; Sc &lt; 900, 180 &lt; We &lt; 550, 1.2 &lt; V₇/V₇ &lt; 1.7</td>
<td>Sh = 0.123Re⁻⁰⁴⁴Sc⁻⁰³⁵We⁻¹⁷⁷(V₇/V₇)⁻¹¹</td>
</tr>
<tr>
<td>Chang and Morsi [20]</td>
<td>Hollow shaft + Rushton turbine</td>
<td>CO</td>
<td>n-hexane</td>
<td>730 &lt; Eu &lt; 10737, 8 &lt; Sc &lt; 487, 1688 &lt; We &lt; 11332, 39506 &lt; Re &lt; 33924</td>
<td>Sh = 3.41 × 10⁻²⁰Re⁻¹³⁶</td>
</tr>
</tbody>
</table>

Table 2

Literature survey on kₗa in GIR
<table>
<thead>
<tr>
<th>Authors</th>
<th>Induction type</th>
<th>Gas</th>
<th>Liquid</th>
<th>Operating conditions</th>
<th>Correlations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chang [21]</td>
<td>Hollow shaft + Rushton turbine</td>
<td>CO, CO&lt;sub&gt;2&lt;/sub&gt;, CH&lt;sub&gt;4&lt;/sub&gt;</td>
<td>n-C6, n-C10, n-C14</td>
<td>546 &lt; Eu &lt; 11320</td>
<td>Sh = 5.114 × 10&lt;sup&gt;-12&lt;/sup&gt; Re&lt;sup&gt;2.18&lt;/sup&gt; Sc&lt;sup&gt;0.63&lt;/sup&gt;Ed&lt;sup&gt;0.28&lt;/sup&gt;Fr&lt;sup&gt;1.73&lt;/sup&gt;</td>
</tr>
<tr>
<td>Chang [21]</td>
<td>Hollow shaft + Rushton turbine</td>
<td>H&lt;sub&gt;2&lt;/sub&gt;</td>
<td>n-C6, n-C10, n-C14</td>
<td>569 &lt; Eu &lt; 10468</td>
<td>Sh = 2.74 × 10&lt;sup&gt;-18&lt;/sup&gt; Re&lt;sup&gt;3.00&lt;/sup&gt; Sc&lt;sup&gt;2.21&lt;/sup&gt;Eu&lt;sup&gt;0.42&lt;/sup&gt;Fr&lt;sup&gt;1.29&lt;/sup&gt;</td>
</tr>
<tr>
<td>Koneripalli et al. [22]</td>
<td>Hollow shaft + Rushton turbine</td>
<td>N&lt;sub&gt;2&lt;/sub&gt;, CO, H&lt;sub&gt;2&lt;/sub&gt;, CO&lt;sub&gt;2&lt;/sub&gt;, CH&lt;sub&gt;4&lt;/sub&gt;</td>
<td>Methanol, ethanol</td>
<td>288 &lt; Eu &lt; 9640</td>
<td>Sh = 4.88 × 10&lt;sup&gt;0&lt;/sup&gt;Re&lt;sup&gt;3.81&lt;/sup&gt; Sc&lt;sup&gt;0.23&lt;/sup&gt; We&lt;sup&gt;4.40&lt;/sup&gt;Ed&lt;sup&gt;0.09&lt;/sup&gt;</td>
</tr>
<tr>
<td>Heim et al. [23]</td>
<td>Hollow shaft</td>
<td>Air, Water, fermentation mixtures</td>
<td></td>
<td>0.28 &lt; Fr&lt;sup&gt;*&lt;/sup&gt; &lt; 1.49</td>
<td>4-pipe impeller: Sh&lt;sup&gt;*&lt;/sup&gt;9.5 × 10&lt;sup&gt;-5&lt;/sup&gt; = 1 - exp(-19.64Re&lt;sup&gt;-0.210&lt;/sup&gt;Fr&lt;sup&gt;-4.336&lt;/sup&gt;)</td>
</tr>
<tr>
<td>Tekie et al. [8]</td>
<td>Hollow shaft + Rushton turbine</td>
<td>N&lt;sub&gt;2&lt;/sub&gt;, O&lt;sub&gt;2&lt;/sub&gt;</td>
<td>Cyclohexane</td>
<td>2100 &lt; We &lt; 13300</td>
<td>Sh = 4.51 × 10&lt;sup&gt;3&lt;/sup&gt;W&lt;sup&gt;-0.21&lt;/sup&gt;Fr&lt;sup&gt;-0.92&lt;/sup&gt;(1 + 1.867 × 10&lt;sup&gt;3&lt;/sup&gt;Ec&lt;sup&gt;-0.3&lt;/sup&gt;)</td>
</tr>
<tr>
<td>Tekie et al. [9]</td>
<td>Hollow shaft + Rushton turbine</td>
<td>N&lt;sub&gt;2&lt;/sub&gt;, O&lt;sub&gt;2&lt;/sub&gt;</td>
<td>Cyclohexane</td>
<td>x&lt;sub&gt;1&lt;/sub&gt;: 6.67 &lt; N &lt; 20.0 Hz</td>
<td>k&lt;sub&gt;L,a&lt;/sub&gt; = 76 ± 21 × 10&lt;sup&gt;8&lt;/sup&gt;(P&lt;sup&gt;-0.80&lt;/sup&gt;V&lt;sub&gt;L&lt;/sub&gt;/L&lt;sup&gt;0.06&lt;/sup&gt;)</td>
</tr>
<tr>
<td>Forrester et al. [24]</td>
<td>Hollow shaft + 6 concave blades</td>
<td>Air, Water</td>
<td></td>
<td>250 &lt; P&lt;sup&gt;*&lt;/sup&gt;/V&lt;sub&gt;L&lt;/sub&gt; &lt; 2250 w/m&lt;sup&gt;3&lt;/sup&gt;</td>
<td>k&lt;sub&gt;L,a&lt;/sub&gt; = 76 ± 21 × 10&lt;sup&gt;8&lt;/sup&gt;(P&lt;sup&gt;-0.80&lt;/sup&gt;V&lt;sub&gt;L&lt;/sub&gt;/L&lt;sup&gt;0.06&lt;/sup&gt;)</td>
</tr>
<tr>
<td>Fillion and Morsi [10]</td>
<td>Hollow shaft + Rushton turbine</td>
<td>N&lt;sub&gt;2&lt;/sub&gt;, H&lt;sub&gt;2&lt;/sub&gt;</td>
<td>Soybean oil</td>
<td>x&lt;sub&gt;1&lt;/sub&gt;: 373 &lt; T &lt; 473 K</td>
<td>N&lt;sub&gt;2&lt;/sub&gt;: ln(k&lt;sub&gt;L,a&lt;/sub&gt;) = -4.86 - 0.179x&lt;sub&gt;1&lt;/sub&gt; + 0.708x&lt;sub&gt;2&lt;/sub&gt; - 0.596x&lt;sub&gt;1&lt;/sub&gt;x&lt;sub&gt;2&lt;/sub&gt; + 0.0759x&lt;sub&gt;1&lt;/sub&gt; + 0.116x&lt;sub&gt;1&lt;/sub&gt;x&lt;sub&gt;2&lt;/sub&gt; - 0.228x&lt;sub&gt;1&lt;/sub&gt;x&lt;sub&gt;2&lt;/sub&gt; - 0.0763x&lt;sub&gt;3&lt;/sub&gt;x&lt;sub&gt;4&lt;/sub&gt; - 0.0754x&lt;sub&gt;1&lt;/sub&gt;x&lt;sub&gt;3&lt;/sub&gt;x&lt;sub&gt;4&lt;/sub&gt; + 0.00269(x&lt;sub&gt;3&lt;/sub&gt;x&lt;sub&gt;4&lt;/sub&gt; + 2.5)e&lt;sup&gt;2.5&lt;/sup&gt; + 1.28 tanh(0.3x&lt;sub&gt;5&lt;/sub&gt;(5 - x&lt;sub&gt;1&lt;/sub&gt;)) + 0.1(2 - 4x&lt;sub&gt;3&lt;/sub&gt;)) - 0.339x&lt;sub&gt;1&lt;/sub&gt;x&lt;sub&gt;2&lt;/sub&gt;x&lt;sub&gt;4&lt;/sub&gt; - 0.339x&lt;sub&gt;1&lt;/sub&gt;x&lt;sub&gt;2&lt;/sub&gt;x&lt;sub&gt;4&lt;/sub&gt;</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>x&lt;sub&gt;2&lt;/sub&gt;: 10 &lt; N &lt; 23.3 Hz</td>
<td>H&lt;sub&gt;2&lt;/sub&gt;: ln(k&lt;sub&gt;L,a&lt;/sub&gt;) = -3.868 + 0.516x&lt;sub&gt;2&lt;/sub&gt; - 0.790x&lt;sub&gt;2&lt;/sub&gt; + 0.223x&lt;sub&gt;2&lt;/sub&gt;&lt;sup&gt;2&lt;/sup&gt; - 0.352x&lt;sub&gt;1&lt;/sub&gt;&lt;sup&gt;2&lt;/sup&gt; + 0.326x&lt;sub&gt;1&lt;/sub&gt;&lt;sup&gt;2&lt;/sup&gt; - 0.00378(x&lt;sub&gt;3&lt;/sub&gt;x&lt;sub&gt;4&lt;/sub&gt; + 3)e&lt;sup&gt;3&lt;/sup&gt; + 2.099 tanh(0.3x&lt;sub&gt;5&lt;/sub&gt;(8 - x&lt;sub&gt;1&lt;/sub&gt;)) + 0.1(2 - 6x&lt;sub&gt;3&lt;/sub&gt;)) - 0.927x&lt;sub&gt;1&lt;/sub&gt;e&lt;sup&gt;-0.2&lt;/sup&gt;</td>
</tr>
</tbody>
</table>
Table 3
Selected literature survey on ANN in the chemical industry

<table>
<thead>
<tr>
<th>Authors</th>
<th>Systems used</th>
<th>Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alvarez et al. [30]</td>
<td>Newtonian and non-Newtonian fluid in bubble columns</td>
<td>Prediction of $k_L a$</td>
</tr>
<tr>
<td>Azlan Hussain [31]</td>
<td>Review</td>
<td>Simulation and online implemention, Kinetic modeling</td>
</tr>
<tr>
<td>Fullana et al. [32]</td>
<td>Supercritical fluid extractors</td>
<td>Prediction of $k_L a$</td>
</tr>
<tr>
<td>García-Ochoa and Gómez Castro [27]</td>
<td>O$_2$/H$_2$O xanthan gum solution in STR</td>
<td>Prediction of $k_L a$</td>
</tr>
<tr>
<td>Henrique et al. [33]</td>
<td>pH neutralization process</td>
<td>Model prediction and simulation, Modeling</td>
</tr>
<tr>
<td>I et al. [34]</td>
<td>Sugar, cell mass, L-lysine</td>
<td>Prediction of $U_{limf}$</td>
</tr>
<tr>
<td>Ilueta et al. [35]</td>
<td>Several system in trickle bed reactors</td>
<td>Prediction of mass transfer coefficient</td>
</tr>
<tr>
<td>Jambunathan et al. [36]</td>
<td>Liquid crystal thermography</td>
<td>Evaluation of heat transfer coefficient</td>
</tr>
<tr>
<td>Krothapally and Palanki [37]</td>
<td>Batch process</td>
<td>Process optimization</td>
</tr>
<tr>
<td>Larachi et al. [38]</td>
<td>3-phase fluidized bed reactor</td>
<td>Simulation of propylene oxidation</td>
</tr>
<tr>
<td>Leib et al. [39]</td>
<td>Fluidized bed</td>
<td>Simulation of propylene oxidation</td>
</tr>
<tr>
<td>Leib et al. [40]</td>
<td>3-phase bubble column</td>
<td>Simulation of propylene oxidation</td>
</tr>
<tr>
<td>Mills et al. [41]</td>
<td>Conical tank, industrial evaporator</td>
<td>Simulation of Fischer-Tropsch process, Control</td>
</tr>
<tr>
<td>Nascimento and Giudici [42]</td>
<td>Nylon-6,6 polymerization</td>
<td>Process optimization</td>
</tr>
<tr>
<td>Nascimento et al. [43]</td>
<td>Chemical process</td>
<td>Optimization</td>
</tr>
<tr>
<td>Nikravesh et al. [44]</td>
<td>CSTR</td>
<td>Control of $h$ and $E_0$</td>
</tr>
<tr>
<td>Qi et al. [45]</td>
<td>Fixed-bed reactor</td>
<td>Prediction of overall heat transfer coefficient, Prediction of $k$</td>
</tr>
<tr>
<td>Reisener et al. [26]</td>
<td>Electrolyte solutions gas sparged reactors</td>
<td>Modeling of Fischer-Tropsch process</td>
</tr>
<tr>
<td>Sharma et al. [46]</td>
<td>H$_2$CO/SiO$_2$–Al$_2$O$_3$ fixed bed reactor</td>
<td>Nonlinear process modeling</td>
</tr>
<tr>
<td>Shaw et al. [47]</td>
<td>Fixed-bed reactor</td>
<td>Predictive control of flow rate and temperature</td>
</tr>
<tr>
<td>Tendulkar et al. [48]</td>
<td>Fixed-bed reactor</td>
<td>Prediction of Nu number, Control</td>
</tr>
<tr>
<td>Thibault and Grandjean [49]</td>
<td>Hybrid process</td>
<td></td>
</tr>
<tr>
<td>Wilson and Zorzetto [50]</td>
<td>Various system in STR</td>
<td></td>
</tr>
<tr>
<td>Zhou et al. [51]</td>
<td>Fixed bed reactor</td>
<td></td>
</tr>
</tbody>
</table>

Table 5
Selected literature on ANN in the chemical industry

Correlation was employed to predict $k_L a$ behavior in different important industrial processes.

2. Neural networks

Traditionally, ANNs have been used to model complex non-linear systems [25,31,32,35,38,40,49] and appeared to be a good alternative to traditional empirical, phenomenological or statistical correlations [25,26,35,38]. The ANNs are more powerful and can manipulate non-linear input–output relationships more successfully than available literature conventional correlations [52].

2.1. Systems studied

A significant number of experimental data (4435 points) were used to develop $k_L a$ neural network correlations. These data were obtained for different gas–liquid systems and cover wide ranges of operating conditions, reactor types (SAR and GIR) and geometries as well as liquid and gas natures, as can be seen in Table 5. The operating conditions used were similar to those employed in industrial processes including, cyclohexane oxidation [8,55], soybean oil hydrogenation [10,57], propylene polymerization [28,54] and Fischer–Tropsch synthesis [14,58]. These data indicate that $k_L a$ values are affected by several variables, which are grouped as follows [59]:

- Geometrical variables: reactor diameter ($D_T$), impeller diameter ($D_{imp}$), and impeller height from the bottom of the reactor ($H_I$).
- Operating variables: reactor mode (SAR, GIR), mixing speed ($N$), liquid height ($H_L$), liquid height above the impeller ($H$), temperature ($T$), and gas partial pressure ($P_g$).
- Physicochemical variables: liquid viscosity ($\mu_L$), liquid and gas densities ($\rho_L$ and $\rho_G$), liquid surface tension ($\sigma_L$) and the gas diffusivity in the liquid ($D_L$).

A dimensional analysis [60] was performed using these variables and 9 dimensionless groups were obtained: $Re$, $Fr$, $Sc$, $We$, $Etu$, $\rho_G/\rho_L$, $D_{imp}/D_T$, $D_{imp}/H_I$ and $D_{imp}/H_L$.

2.2. BPNNs

Two BPNNs, one dimensional and one dimensionless, each with its own input were constructed. The inputs to the dimensional BPNN were the geometrical, operating and physicochemical variables as shown in Table 6a, whereas the inputs to the dimensionless BPNN were the dimensionless groups as presented in Table 6b. An additional input, the ‘reactor operating mode’, was added in both BPNNs as shown in these tables.

2.2.1. Model and architecture

The critical step in building a robust ANN is to create an architecture, which should be as simple as possible and has a fast capacity for learning the data set. The robustness of the ANN will be the result of the complex interactions between its topology and the learning
scheme. The choice of the input variables is the key to insure complete description of the systems, whereas the quality as well as the number of the training observations (experimental data) have a tremendous impact on both the reliability and performance of the ANN. The two BPNNs used were constructed as follows:

1. One input layer; one output node; two hidden layers; all neurons were interconnected and all connections were weighted.
2. Each neuron possessed a bias.
3. The transfer function was a sigmoid of the form:

\[ F(x) = \frac{1}{1 + \exp(-x)} \] (1)

The basic architecture of the BPNNs is given in Fig. 1. The number of neurons, \((n)\) and \((m)\) in the first and second hidden layers were determined based on the analysis of errors during the training step of the networks. The PITTNET software developed at the University of Pittsburgh was used to build and validate the two created BPNNs. The matrix formulation for the calculation methodology is briefly described in the Appendix B.

2.2.2. Training or learning phase: back-propagation algorithm

The learning algorithm for the back-propagation, which is commonly accepted [61–63], was used for the development of the ANNs. In this algorithm, the training was supervised by means of a known output data set and the connection weights were adjusted according to the gradient descent method, as the mean squared error (MSE) was minimized towards the smallest error possible [61–63]. More precisely, the training data were fed forward leading to the calculation of the output and associated errors. Then, the associated errors were back-propagated and the adjustment of the weights was completed accordingly [52,61–63]. This process was repeated until the MSE between the experimental and calculated \((k_{i,a})\) values was less than the chosen tolerance \((10^{-7})\). The mean absolute errors \((MAE)\), the root mean squared errors \((RMSE)\) and the \(R^2\) values were also calculated and used in the validation and construction procedures. Additional details of the back-propagation algorithm are given in Fig. 2. It should be noted that two phenomena were taken into consideration during the construction and validation of the BPNNs. The first phenomenon is over-training, mainly attributed to a large number of iterations, which generally leads to an excellent prediction of the training data set, while predicting poorly the untrained values.

<table>
<thead>
<tr>
<th>Authors</th>
<th>System studied IU</th>
<th>Reactor type</th>
<th>Output parameters</th>
<th>ANN type and topology</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alvarez et al. [30]</td>
<td>CO(_2)/Sucrose and CMC</td>
<td>Bubble column</td>
<td>(k_{i,a})</td>
<td>BPN-FF</td>
</tr>
<tr>
<td>García-Ochoa and Gómez Castro [27]</td>
<td>O(_2)/H(_2)/O xanthan gum sol.</td>
<td>Baffled stirred tank</td>
<td>(k_{i,a})</td>
<td>FF-ML 13-4-1</td>
</tr>
<tr>
<td>Iliuta et al. [35]</td>
<td>805 (\leq \mu_L \leq 1450)</td>
<td>Trickle beds</td>
<td>(Sh_{G}), (Sh_{L}) and (a , dv/(1 - e))</td>
<td>FF-ML 7-13-1, 7-8-1, 8-11-1</td>
</tr>
<tr>
<td>Larachi et al. [38]</td>
<td>780 (\leq \mu_L \leq 1623)</td>
<td>3-Phase fluidized beds</td>
<td>(U_{Lmf}), (Re_L)</td>
<td>FF-ML 8-6-1, 5-9-1</td>
</tr>
<tr>
<td>Leib et al. [39]</td>
<td>Propylene oxidation process</td>
<td>Fluidized bed</td>
<td>(U_{b,bo}), (y_{i,bo}), (y_{4-6}), (w_{i4}), (w_{4-6})</td>
<td>FF-ML 11-8-9</td>
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<tr>
<td>Reisener et al. [26]</td>
<td>Electrolyte solution</td>
<td>Slurry bubble column</td>
<td>(C_{Go}), (C_L), (U_G)</td>
<td>FF-ML 6-5-3</td>
</tr>
<tr>
<td>Sharma et al. [46]</td>
<td>H(_2)O/CO/SiO(_2)/Al(_2)O(_3)</td>
<td>Fixed bed</td>
<td>(h) and (E_0)</td>
<td>DNNC-FF</td>
</tr>
<tr>
<td>Qi et al. [45]</td>
<td>O(_2)/Benzene/V(_2)O(_5)</td>
<td>Fixed-bed</td>
<td>Heat transfer coefficient</td>
<td>FF-ML, 3 ILN and 1 OLN</td>
</tr>
<tr>
<td>Yang et al. [25]</td>
<td>0 (\leq P/V_L \leq 55000)</td>
<td>Fixed bed</td>
<td>Phenol flow rate and T</td>
<td>FF-ML, 6-11-1</td>
</tr>
<tr>
<td></td>
<td>0.8 (\leq \mu_L \leq 70.2)</td>
<td>Stirred tank</td>
<td>(k_{i,a})</td>
<td>FF-ML, 6-11-1</td>
</tr>
<tr>
<td>Authors</td>
<td>Number of data points</td>
<td>Liquid</td>
<td>Gas</td>
<td>$T$, K</td>
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<td>--------------</td>
<td>-----------------------</td>
<td>-------------------------</td>
<td>----------------------</td>
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</tr>
<tr>
<td>Chang [21]</td>
<td>272</td>
<td>Water</td>
<td>N₂</td>
<td>328–378</td>
</tr>
<tr>
<td>Chang [21]</td>
<td>274</td>
<td>n-hexane</td>
<td>H₂</td>
<td>328–378</td>
</tr>
<tr>
<td>Chang [21]</td>
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<td>n-decane</td>
<td>H₂</td>
<td>328–378</td>
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<tr>
<td>Chang [21]</td>
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<td>n-tetrade-cane</td>
<td>H₂</td>
<td>328–378</td>
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<tr>
<td>Koneripalli [53]</td>
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<td>Methanol</td>
<td>N₂</td>
<td>328–428</td>
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<tr>
<td>Koneripalli [53]</td>
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<td>Ethanol</td>
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<tr>
<td>Li [54]</td>
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<td>H₂</td>
<td>297–333</td>
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<td>H₂</td>
<td>313–353</td>
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<td>Mizan [5]</td>
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<td>n-hexane</td>
<td>C₂H₆</td>
<td>313–353</td>
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Table 5 (Continued)

<table>
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<th>Authors</th>
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<th>Gas</th>
<th>T, K</th>
<th>P1, bar</th>
<th>Reactor mode</th>
<th>N, rpm</th>
<th>DT, m</th>
<th>Dimp, m</th>
<th>HL, m</th>
<th>HF, m</th>
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<tbody>
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<td>2.4–16.2</td>
<td>SAR</td>
<td>800–1200</td>
<td>0.125</td>
<td>0.0508</td>
<td>0.198–0.225</td>
<td>0.0670</td>
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<tr>
<td>Tekie [55]</td>
<td>398</td>
<td>C6H12</td>
<td>N2, O2</td>
<td>330–340</td>
<td>5.8–34.1</td>
<td>SAR and GIR</td>
<td>400–1200</td>
<td>0.115</td>
<td>0.0508</td>
<td>0.171–0.268</td>
<td>0.0635</td>
</tr>
<tr>
<td>Mohammad [56]</td>
<td>235</td>
<td>Benzoic acid</td>
<td>O2</td>
<td>473</td>
<td>0.9–5.0</td>
<td>SAR and GIR</td>
<td>1000</td>
<td>0.076</td>
<td>0.0317</td>
<td>0.108</td>
<td>0.0413</td>
</tr>
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<td>Fillion [57]</td>
<td>654</td>
<td>Soybean oil</td>
<td>H2, N2</td>
<td>373–473</td>
<td>1.0–5.0</td>
<td>SAR and GIR</td>
<td>600–1400</td>
<td>0.115</td>
<td>0.0508</td>
<td>0.171–0.268</td>
<td>0.0635</td>
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Table 6a, b
Ranges of the BPNNs input parameters used in this study

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<tr>
<th>Ymax (ln kL,λmax)</th>
<th>Ymax (ln kG,λmax)</th>
<th>ρL, kg m⁻³</th>
<th>ρG, kg m⁻³</th>
<th>10⁻⁵ × μL, N s m⁻²</th>
<th>10⁻⁵ × μG, N m⁻¹</th>
<th>10⁻⁹ × Dλ, m s⁻¹</th>
<th>P1, bar</th>
<th>Reactor mode</th>
<th>N, rpm</th>
<th>DT, m</th>
<th>Dimp, m</th>
<th>HL, m</th>
<th>HF, m</th>
</tr>
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<tbody>
<tr>
<td>Ranges 6a</td>
<td>–0.495</td>
<td>–7.729</td>
<td>309.9–1011.1</td>
<td>0.05–0.27</td>
<td>5.0–668.3</td>
<td>1.2–64.5</td>
<td>3.5–153.9</td>
<td>0.86–59.59</td>
<td>0 = SAR</td>
<td>400–1400</td>
<td>0.406–0.500</td>
<td>0.237–0.444</td>
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</tbody>
</table>

Ranges 6b

<table>
<thead>
<tr>
<th>Ymax (log Sh,λmax)</th>
<th>Ymax (log Sh,λmax)</th>
<th>Re</th>
<th>Sc</th>
<th>Eu</th>
<th>We</th>
<th>Fr</th>
<th>ρG/ρL</th>
<th>Reactor mode</th>
<th>H2/DT</th>
<th>D3/Dimp</th>
<th>H3/Dimp</th>
</tr>
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<tbody>
<tr>
<td>Ranges 6b</td>
<td>5.456</td>
<td>2.088</td>
<td>5571–445 836</td>
<td>0.88–1274.1</td>
<td>85–41 876</td>
<td>285–18 949</td>
<td>0.23–3.52</td>
<td>6.4 × 10⁻⁵</td>
<td>0 = SAR</td>
<td>1.05–1.49</td>
<td>2–2.46</td>
</tr>
<tr>
<td></td>
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<td></td>
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<td></td>
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<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

1 = GIR
The second phenomenon is under-training, which interpolates the untaught values relatively well, while predicting poorly the training data set.

3. Results and discussions

3.1. Architectures choices

All the experimental \( k_{1,\alpha} \) data points collected were used to build and validate the ANN correlations. In the training algorithm of the BPNNs, the MSE was minimized for each epoch, i.e. iteration. As depicted in Fig. 3, the error appears to decrease with increasing the number of hidden layers and neurons. A minimum error was found for a network topology of 10-23-23-1 and 10-30-30-1 for the dimensional and dimensionless BPNN, respectively. Fig. 3 also shows that the relative error between the networks does not significantly decrease after corresponding topologies of 10-10-1 and 10-15-1. It is important to mention that topologies of 10-23-23-1 and 10-30-30-1 possess a significant number of parameters, 829 and 1291, respectively, representing roughly 1/5 of the data used in the training step. The choice of such topologies could lead to an over-training of the BPNNs and consequently will reduce their ability to accurately interpolate \( k_{1,\alpha} \) values. On the other hand, the topologies of 10-10-1 and 10-15-1, with only 121 and 181 parameters, appear to be the optimal choice for the construction of the dimensional and dimensionless...
BPNNs, respectively. It should also be mentioned that a learning rate of 0.25 as suggested in Refs. [52,61–63] was chosen with 10000 epochs, since as shown in Fig. 4 the MAE and MSE sensibly decrease with the number of iterations. The weights of the two constructed BPNNs are given in Tables 7 and 8.

3.2. Validation of the BPNNs

In the validation step, since the ANN acts as a ‘Black Box’ and it is almost impossible to determine why a specific BPNN would provide acceptable predictions, two different steps were followed to overcome such a problem. In the first step, cross validation method was used [64,65], where numerous sub-networks with identical architecture and parameters were built and trained using all the experimental data. In the second step, these sub-networks were tested using the untaught \( k_{La} \) values by Inga [58] and Martinez [66], as their studies were conducted with different gas–liquid systems, reactors geometries and operating conditions. Fig. 5 shows that the prediction of these untaught \( k_{La} \) values using the dimensional BPNN is acceptable with \( R^2 \) of 86% and standard deviation of 41%, whereas those for the dimensionless BPNN are 87 and 61%, respectively. This large standard deviation for the dimensionless BPNN could be related to the over-training of this BPNN and/or the inability of dimensionless numbers in providing accurate influence of all variables involved.

3.3. Predictions of \( k_{La} \) values using BPNNs

Fig. 6a and b shows that the dimensional and dimensionless BPNNs can predict \( k_{La} \) values with \( R^2 \) of 90.5 and 88.6%, and corresponding standard deviations of 23.3 and 24.1%, respectively. Figs. 7 and 8 compare the experimental \( k_{La} \) values with the predictions of the dimensionless correlations proposed by Wu [7] and Tekie et al. [8] in the SAR, and Chang [21] and Forrester et al. [24] in the GIR. From Figs. 6–8, it appears that the BPNN correlations provide good predictions, whereas the correlations by Wu [7], Tekie et al. [8], Chang [21] and Forrester et al. [24] fail to satisfactorily predict the majority of the experimental \( k_{La} \) values used in this study. This was expected since their correlations did not consider several important parameters, such as gas density, liquid surface tension or reactor geometry, whose influences on \( k_{La} \) are obviously significant.

Since acceptable agreements in both the validation and prediction steps were obtained with the dimensional BPNN, 3-dimensional response surfaces were generated and used to study the effect of liquid physicochemical
Fig. 4. Error analysis on the BPNNs as function of the epochs.

Table 7
Weights and biases of the 10-10-1 dimensional BPNN

<table>
<thead>
<tr>
<th>Input weights $u_{ij}$</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-0.08</td>
<td>-6.61</td>
<td>-1.49</td>
<td>4.08</td>
<td>12.54</td>
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<td>1.92</td>
<td>-1.11</td>
<td>-0.73</td>
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</tr>
<tr>
<td>2</td>
<td>-0.52</td>
<td>-4.06</td>
<td>4.71</td>
<td>3.25</td>
<td>-2.48</td>
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<tr>
<td>3</td>
<td>1.85</td>
<td>0.15</td>
<td>-2.55</td>
<td>-1.17</td>
<td>-5.97</td>
<td>-3.59</td>
<td>-2.24</td>
<td>-2.30</td>
<td>-2.71</td>
<td>19.13</td>
</tr>
<tr>
<td>4</td>
<td>2.08</td>
<td>2.18</td>
<td>0.32</td>
<td>1.21</td>
<td>5.10</td>
<td>-0.60</td>
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<td>-1.43</td>
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<td>-6.35</td>
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<tr>
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<td>-2.68</td>
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<td>-4.08</td>
<td>-2.03</td>
<td>7.08</td>
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<td>7</td>
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<td>1.30</td>
<td>-1.82</td>
<td>0.22</td>
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<td>-4.97</td>
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<table>
<thead>
<tr>
<th>Bias of hidden layer $u_{b,i}$</th>
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<th>-1.92</th>
<th>-2.53</th>
<th>0.34</th>
<th>1.20</th>
<th>-8.69</th>
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<td>7</td>
<td>8</td>
<td>9</td>
<td>10</td>
<td></td>
</tr>
</tbody>
</table>

| Output weights $w_{i}$ | 1.68 | 2.83 | -2.15 | -2.84 | -2.97 | -4.25 | 4.30 | 1.50 | 4.67 | -2.77 |
| Bias of output neuron $w_0$ | -2.33 |

Fig. 4. Error analysis on the BPNNs as function of the epochs.
Table 8
Weights and biases of the 10-15-1 dimensionless BPNN

<table>
<thead>
<tr>
<th></th>
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<tbody>
<tr>
<td>Input weights $u_{ij}$</td>
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<td>-7.65</td>
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<tr>
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<td>-2.52</td>
<td>10.15</td>
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<td>-1.38</td>
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<td>-3.68</td>
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<td>7.03</td>
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<td>-13.77</td>
<td>3.82</td>
<td>-6.78</td>
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3.4. Effects of liquid physicochemical properties on $k_{La}$

Fig. 9a and b illustrates the effect of liquid viscosity on $k_{La}$ in the SAR and GIR, respectively. This is similar to the increase of liquid viscosity due to chemical reactions as in Fischer–Tropsch synthesis or hydrogenation of vegetable oil processes. As it can be observed in Fig. 9a, $k_{La}$ decreases slightly with increasing liquid viscosity in the SAR, which is in agreement with literature data [3,4]. In the SAR, the gas–liquid interfacial area can be considered almost constant and accordingly the decrease of $k_{La}$ with increasing viscosity can be attributed to the decrease of the mass transfer coefficient, $k_L$. In fact, an increase of the viscosity has been reported to decrease the turbulences at the gas–liquid surface leading to a decrease of the surface renewal rate and consequently $k_L$ [10,55,67,68]. In the GIR, the gas–liquid interfacial area is not constant as gas bubbles are induced into the liquid when operating above the critical mixing speed for gas induction [69]. In a GSR, Rushton and Bimbinet [70] for water/corn syrup solution found that the gas holdup increases with liquid viscosity for $\mu_L$ values less than $5 \times 10^{-3}$ Pa.s and then decreases with further increase in liquid viscosity. In a GIR, for water/CMC solution He et al. [71] reported similar findings which were attributed to the effect of liquid viscosity on the induced gas flow rate as described by Aldrich and van Deventer [72] and Fillion et al. [69]. Vermulen et al. [73] reported a rather slight decrease of the break-up rate, i.e. increase of the bubble coalescence with increasing liquid viscosity. Thus, if the effect of liquid viscosity on the gas holdup is stronger than that on the bubble size, the gas–liquid interfacial area, $a$ is expected to increase and then decrease with increasing liquid viscosity. This means that increasing liquid viscosity could increase and decrease $k_{La}$ due its resultant effect of $a$ and $k_L$. In this study, the behavior of $k_{La}$ follows that of $k_L$ in the SAR, whereas in the GIR $k_{La}$ is primarily affected by $a$ rather than $k_L$, as can be seen in Fig. 9a and b, respectively.

Fig. 10a and b depicts the effect of liquid surface tension on $k_{La}$ in the SAR and GIR. This figure could be used to speculate the effect of surface-active agents and impurities on $k_{La}$ in biochemical processes. Fig. 10a
Fig. 6. Comparison between experimental and predicted $k_{1,a}$ values of the BPNNs.

Dimensional BPNNs
Topology: 10-10-1
$R^2$: 90.5%

Dimensional BPNNs
Topology: 10-15-1
$R^2$: 88.6%

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Chang [21]
Mizan [5]
Koneripalli [53]
Li [54]
Tekie [55]
Mohammad [56]
Fillion [57]
Fig. 7. Comparison between experimental and predicted $k_La$ values from literature correlations in SAR.

Wu [7]

\[
k_La = 6.34 \times 10^{-2} \left( \frac{P^*}{V_L} \right)^{0.65}
\]

Tekie [8]

\[
Sh = 4.51 \times 10^3 We^{-0.21} Fr^{0.92}
\]
Fig. 8. Comparison between experimental and predicted $k_L\alpha$ values from literature correlations in GIR.

- **Forrester et al. [24]**
  
  $k_L\alpha = (76 \pm 21) \times 10^{-6} \left( \frac{P_r}{V_L} \right)^{0.802 \pm 0.06}$

- **Chang [21]**
  
  $Sh = 2.74 \times 10^{-18} Re^{3.00} Sc^{2.21} Eu^{-0.42} We^{1.29}$
shows that \( k_{L,a} \) values obtained in the SAR increase with increasing liquid surface tension, which follows the behavior of \( k_L \) reported by Levich [74] and Davies [67], particularly under high turbulent conditions. In the GIR, \( k_{L,a} \) was found to slightly decrease with increasing liquid surface tension as illustrated in Fig. 10b. Calderbank [75] and Hinze [76] found that increasing liquid surface tension substantially increases the average bubble size in agitated reactors, which was found to decrease the gas holdup as reported by He et al. [71] and Albal et al. [3] in the GIR, and Calderbank [75] in the GSR. This means that although increasing liquid surface tension increases \( k_L \), it decreases the gas–liquid interfacial area, which agrees with the findings by Patwardhan et al. [77] in the GIR and Calderbank [75] in the GSR. As a result of this behavior, \( k_{L,a} \) could decrease or increase with increasing liquid surface tension in the GIR. In this study, the effect of liquid surface tension on \( a \) appears to be stronger than that on \( k_L \) leading to an increase of \( k_{L,a} \) with liquid surface tension in the GIR, as can be seen in Fig. 10b.

Fig. 11a and b shows the effect of liquid density on \( k_{L,a} \) in the SAR and GIR as an attempt to simulate the effect of changing liquid density during polymerization processes. As can be observed in this figure, \( k_{L,a} \) values seem to decrease with increasing liquid density in both reactor types. The available literature on the effect of liquid density on the mass transfer coefficient, however, is somewhat contradictory. For instance, Davies [67], Kosinski et al. [78] and Calderbank and Moo-Young [68] developed correlations where \( k_L \) is proportional to the liquid density to a power ranging from 1/4 to 1/2; however, Farritor and Hughmark [79], Boussinesq [80] and Higbie’s penetration theory [81] reported no effect of liquid density on \( k_L \). Furthermore, Zlokarnik [82], Aldrich and van Deventer [72] and Joshi and Sharma [11] studied the effect of liquid density on the induced gas flow rate in the GIR and concluded that an increase of liquid density resulted in an enhancement of the buoyancy forces acting on the gas bubbles which led to a decrease of the induced gas flow rate. This decrease of the induced gas flow rate with liquid density in the GIR decreases the gas holdup and subsequently the gas–liquid interfacial area. Therefore, it seems that \( k_{L,a} \) values decrease with increasing liquid density as a result of the decrease of the gas–liquid interfacial area in the GIR as illustrated in Fig. 11b. From the similarity of the \( k_{L,a} \) trends in both reactor types, however, it might be
inferred that the decrease of $k_{L}a$ with increasing liquid density, observed in Fig. 11a, could be the result of decreasing bubble entrainment in the SAR, which was reported to occur by few investigators [2,3]. Nonetheless, it can be concluded that increasing liquid density decreases $k_{L}a$ as it affects primarily the gas–liquid interfacial area rather than $k_{L}$ in both reactor types.

Fig. 12a and b shows the effect of diffusivity on $k_{L}a$ in the SAR and GIR which can be used to compare the effect of hydrogen and carbon dioxide diffusivities on $k_{L}a$ in Fischer–Tropsch synthesis. In both reactor types, $k_{L}a$ values were found to increase with increasing gas diffusivity, which is in accord with several literature findings [4,67,68,74,80,81,83]. For instance, Beenackers and van Swaaij [83] reported that $k_{L}$ is proportional to the diffusivity to a power ranging from 0.5 for the penetration theory and 1.0 for the film model. Thus, it can be concluded that $k_{L}a$ increases with the diffusivity due to the increase of $k_{L}$, since the diffusivity is presumably independent of the gas–liquid interfacial area in both reactor types.

3.5. Effects of operating variables on $k_{L}a$

Figs. 9–11a and b illustrate the effect of mixing speed on $k_{L}a$ in the SAR and GIR under operating conditions typical to different industrial processes. In agreement with the available literature on the SAR and GIR [2–13], $k_{L}a$ was found to increase with mixing speed. In the SAR, the interfacial area can be considered almost constant, and therefore the increase of $k_{L}a$ with $N$ can essentially be attributed to the increase of $k_{L}$. Increasing $N$ intensifies the turbulences and thus the surface renewal rate [10,55,79,83], which increases the mass transfer coefficient in the SAR. In the GIR, the gas–liquid interfacial area is not constant, since at the critical mixing speed for gas induction gas bubbles are induced into the liquid [69]. Above this critical mixing speed, further increase of $N$ increases the induced gas flow rate [69,71,72], which increases the gas holdup [69,72] and the corresponding gas–liquid interfacial area [72]. Thus, both $a$ and $k_{L}$ and subsequently $k_{L}a$ values increase with mixing speed in the GIR. It should be mentioned,
Fig. 13. Effect of reactor geometry on $k_L\alpha$ values in SAR and GIR.

3.6. Effects of reactor geometry and operating mode on $k_L\alpha$

Fig. 13a and b presents the effect of $D_{\text{imp}}/D_T$ (impeller/reactor diameter ratio) and $H_T/H_L$ (impeller height from the bottom of the reactor/liquid height ratio) on $k_L\alpha$ for $O_2$ in water in the SAR and GIR, and as can be seen, $k_L\alpha$ appears to increase with both ratios in the SAR, which is in agreement with the available literature [90–92]. It is generally accepted that an increase of $D_{\text{imp}}/D_T$ and $H_T/H_L$ intensifies the turbulences at the gas–liquid surface, which leads to an increase of the surface renewal rate and thus $k_L$ [74,79]. Under specific conditions, on the other hand, increasing both these ratios can result in an enhancement of surface entrainment in the SAR, which further increases the gas–liquid interfacial area [2,3]. Therefore, both $a$ and $k_L$ and subsequently $k_L\alpha$ increase with increasing $D_{\text{imp}}/D_T$ and $H_T/H_L$ in the SAR. In the GIR, similar results are observed as shown in Fig. 13b. In fact, an increase of $D_{\text{imp}}/D_T$ and $H_T/H_L$ leads to an increase of the pumping capacity of the impeller, which results in an increase of the induced gas flow rate and subsequently the gas holdup [11,69,71]. This increase of gas holdup produces higher gas–liquid interfacial area, which in conjunction with an increase of $k_L$ provides higher $k_L\alpha$ values in the GIR.

Figs. 9–13a and b depict the effect of reactor operating mode on $k_L\alpha$ for typical gases in a Fischer–Tropsch liquid, olefinic medium, vegetable oil and water. As can be observed in these figures, $k_L\alpha$ values were found to be greater in the GIR than in the SAR. In fact, in the GIR above the critical mixing speed for gas induction [69], gas bubbles are induced in the liquid phase which creates additional gas–liquid interfacial area leading to higher $k_L\alpha$ values than those in the SAR [10,55].

4. Conclusions

This study has demonstrated the potential of using ANNs as a correlation/prediction tool for $k_L\alpha$ in SARs and GIRs. Using a large number of experimental data points (4435), one dimensional and one dimensionless BPNNs were constructed and successfully correlated $k_L\alpha$ values of typical industrial processes under wide ranges of operating conditions. Due to its acceptable predictions, the dimensional BPNN was used to simulate and study the effect of physicochemical properties, operating conditions and reactor geometrical parameters on $k_L\alpha$ in multiphase processes. The analysis of the predicted results led to the following conclusion:

1) Increasing liquid viscosity (such as in Fischer–Tropsch synthesis or hydrogenation of vegetable oil process due to chemical reaction) appeared to decrease $k_L\alpha$ values in the SAR. In the GIR,
however, increasing liquid viscosity was found to increase and then decrease $k_{L}a$ values.

2) Increasing liquid density (such as in polymerization processes) resulted in a decrease of $k_{L}a$ values in both reactor types.

3) Increasing liquid surface tension (such as in biochemical processes) was found to decrease $k_{L}a$ in the GIR. In the SAR, however, increasing liquid surface tension appeared to increase $k_{L}a$ values.

4) Increasing gas diffusivity and partial pressure (such as in Fischer–Tropsch synthesis) resulted in an increase of $k_{L}a$ values in both reactor types.

5) $k_{L}a$ values appeared to increase with increasing mixing speed, and with $D_{imp}/D_{T}$ as well as $H_{T}/H_{L}$ in the SAR and GIR for all the processes utilized in this study.

6) $k_{L}a$ values in the GIR appeared to be always higher than those in the SAR due to the increase of gas–liquid interfacial area in all the processes used in this study.

Even though the ANNs appeared to be a viable optimization and scale-up tool for industrial reactors, it should be mentioned that the use of a larger $k_{L}a$ database could further improve their predictive accuracy.

**Appendix A: Nomenclature**

- $a$: interfacial area (m$^{-1}$)
- $C_{G}$: gas phase concentration (kmol·m$^{-3}$)
- $C_{L}$: liquid phase concentration (kmol·m$^{-3}$)
- $D_{A}$: diffusivity (m$^{2}$·s$^{-1}$)
- $D_{imp}$: impeller diameter (m)
- $D_{T}$: reactor diameter (m)
- $d_{p}$: particle diameter (m)
- $d_{c}$: sauter mean particle diameter (m)
- $E_{0}$: activation energy (J)
- $H$: liquid height above the impeller (m)
- $H_{imp}$: impeller height (m)
- $H_{b}$: baffles height (m)
- $H_{L}$: liquid height (m)
- $h_{f}$: height between the tank and impeller bottom (m)
- $h$: heat transfer coefficient (J·K$^{-1}$·m$^{-2}$·s$^{-1}$)
- $k_{L}$: mass transfer coefficient (m·s$^{-1}$)
- $k_{L}a$: volumetric mass transfer coefficient (m·s$^{-1}$)
- $N$: mixing speed (rpm or Hz)
- $P_{1}$: gas partial pressure (bar)
- $P^*$: power input (W)
- $R^2$: regression coefficient (%) $\left(100 \text{%}\right)$
- $T$: temperature (K)
- $w_{i,j}$: bias of the $i$th hidden neuron $\left(-\right)$
- $w_{0}$: bias of the output neuron $\left(-\right)$
- $w_{i,j}$: weight between the $i$th input neuron and the $j$th hidden neuron $\left(-\right)$
- $w_{0,i}$: weight between the $i$th hidden neuron and the output neuron $\left(-\right)$
- $w_{i}$: molar fraction of the compound $i$ in the emulsion Tables 3 and 4 $\left(-\right)$
- $x_{10}$: normalized input vector
- $x_{i}$: coded variable for $T$ $\left(-\right)$
- $x_{2}$: coded variable for $N$ $\left(-\right)$
- $x_{3}$: coded variable for $P$ $\left(-\right)$
- $x_{4}$: coded variable for $H$ $\left(-\right)$
- $y_{pred}$: net input signal of the output neuron $\left(-\right)$
- $y_{max}$: maximum value of the trained output data set $\left(-\right)$
- $y_{min}$: minimum value of the trained output data set $\left(-\right)$
- $y_{out}$: output signal of the output neuron $\left(-\right)$
- $y_{i}$: molar fraction of the compound $i$ in the bubbles Table 3 and Table 4 $\left(-\right)$
- $z_{pred}$: net input signal of the $i$th hidden neuron $\left(-\right)$
- $z_{out}$: output signal of the $i$th hidden neuron $\left(-\right)$

**Greek letters**

- $\varepsilon$: porosity of the fixed bed $\left(-\right)$
- $\varepsilon_{L}$: gas holdup $\left(-\right)$
- $\mu$: viscosity (kg·m$^{-1}$·s$^{-1}$ or Pa·s)
- $\rho$: density (kg·m$^{-3}$)
- $\sigma$: surface tension (N·m$^{-1}$)
- $\sigma$: standard deviation: $\sigma = 100 \times \sqrt{\frac{1}{N-1} \sum_{i=1}^{N} (y_{pred,i} - \bar{y})^2}$ (%)

**Abbreviations**

- ANN: artificial neural network
- BPNN: back-propagation neural network
- DNN: dynamic neural network control
- FF: feed forward
- GIR: gas inducing reactor
- GSR: gas sparging reactor
- HLN: hidden layer neurons
- ILN: input layer neurons
- IU: international unit
- MAE: mean absolute error
- ML: multi-layer
- MSE: mean squared error
- OLN: output layer neurons
- RMSE: root mean squared error
- SS conc: steady state concentration, (g/Nm$^{3}$ of H$_{2}$+CO)

**Indices**

- $L$: liquid phase
- $G$: gas phase
- $S$: solid phase

**Dimensionless numbers**

- $E_{u}$: Euler number
- $F_{r}$: Froude number
- $F_{r}^*$: modified Froude number
- $R_{e}$: Reynolds number
- $R_{e}^*$: Reynolds number (bubble or particle)
- $S_{c}$: Schmidt Number
- $S_{h}$: Sherwood number
- $S_{h}^*$: modified Sherwood number (bubble or particle)
- $W_{e}$: Weber number

$$\frac{P_{1}}{\mu_{L} \mu_{B}} \left(\frac{D_{imp}^{2} \times \rho_{L} \times N^{2}}{D_{T} \times \rho_{B}}\right)$$
Appendix B: Calculation procedure of the output signal

1. The net input to \((Z_1)\) is denoted \((z_1)\) and is calculated as follow:
\[
(z_1) = (u_0) + [u](x_{10})
\]
(2)

The matrix \([u]\) consists of \(n\) rows and 10 columns, corresponding to the number of input variables and nodes in the hidden layer 1:

\[
[u] = \begin{bmatrix}
  u_{1,1} & u_{1,2} & \ldots & \ldots & u_{1,10} \\
  u_{2,1} & u_{2,2} & \ldots & \ldots & u_{2,10} \\
  \vdots & \vdots & \ddots & \ddots & \vdots \\
  \vdots & \vdots & \ddots & \ddots & \vdots \\
  u_{n,1} & u_{n,2} & \ldots & \ldots & u_{n,10}
\end{bmatrix}
\]

(3)

It is also important to mention that each value of each input vector \(x_{10}\) was normalized as follows:

\[
\text{Normalized value} = \frac{\text{Actual value} - \text{Minimum value of the data set}}{\text{Maximum value of the data set} - \text{Minimum value of the data set}}
\]

(4)

2. The activation function is applied to \((z_1)\) to calculate the node output signal denoted \((Z_1)\):
\[
Z_1 = F(z_1)
\]
(5)

3. The net input to \((Z_2)\) is denoted \((z_2)\) and is calculated from the output signal, \((Z_1)\):
\[
z_2 = (v_0) + [v](Z_1)
\]
(6)

The matrix \([v]\) consists of \(m\) rows and \(n\) columns, corresponding to the number of nodes in the hidden layer 2 and 1:

\[
[v] = \begin{bmatrix}
  v_{1,1} & v_{1,2} & \ldots & \ldots & v_{1,n} \\
  v_{2,1} & v_{2,2} & \ldots & \ldots & v_{2,n} \\
  \vdots & \vdots & \ddots & \ddots & \vdots \\
  \vdots & \vdots & \ddots & \ddots & \vdots \\
  v_{m,1} & v_{m,2} & \ldots & \ldots & v_{m,n}
\end{bmatrix}
\]

(7)

4. As in 2, the activation function is applied to \((z_2)\) to calculate the node output signal of the hidden layer 2, denoted \((Z_2)\):
\[
Z_2 = F(z_2)
\]
(8)

5. The net input to \((Y_{\text{pred}})\) is denoted \((y_{\text{pred}})\) and is calculated from the output signal, \((Z_2)\) and the output weights, \([w]\), as follow:
\[
y_{\text{pred}} = w_0 + [w](Z_2)
\]
(9)

In this study, the output matrix of the weights consists of 1 row and \(m\) columns

Finally, the activation function is applied again to \(y_{\text{pred}}\) to calculate the output value, \(Y_{\text{pred}}\):
\[
Y_{\text{pred}} = F(y_{\text{pred}})
\]
(10)

In addition, since the PITTNET program normalizes all vectors, the outputs (target) for the dimensional and dimensionless BPNNs, \(\ln(k_{L}d)\) and \(\log(S\bar{h})\) respectively, were calculated as follows:

\[
\ln(k_{L}d) \text{ or } \log(S\bar{h}) = \frac{Y_{\text{pred}}}{(Y_{\text{max}} - Y_{\text{min}}) + Y_{\text{min}}}
\]
(11)

With \(Y_{\text{max}}\) and \(Y_{\text{min}}\) given in Table 6.

References
