



Development of a multiscale model for the design and scale-up of gas/liquid stirred tank reactors

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HIGHLIGHTS

- A multiscale model is developed as a tool for the design and scale-up of gas/liquid STRs.
- It combines a compartmental model, a simplified CFD model and theoretical correlations.
- It is shown to predict adequately the mean $k_L a$ value of each compartment.
- The effects of operating conditions and scale-up on the compartmental values of $k_L a$ are analyzed.

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ABSTRACT

A multiscale gas/liquid flow model was developed as a tool for the design and scale-up of stirred tank reactors (STRs). The model is based on the compartmentalization of the STR into zones and the use of simplified less computationally intensive gas/liquid flow simulations. It predicts the mean value of the local volumetric mass transfer coefficient ($k_L a$) in each compartment based on the local hydrodynamic parameters therein (i.e., gas hold-up and liquid turbulent energy dissipation rate). The adequacy of the model at each step was carefully assessed using experimental data drawn from the literature. The proposed model was able to predict the overall volumetric mass transfer coefficient in STRs agitated with a Rushton turbine with good adequacy. The effects of operating conditions and scale-up on the distribution of $k_L a$ were also studied. The contributions of each compartment to the overall mass transfer inside the STR could be changed considerably by altering the operating conditions and scale-up. It was estimated that by increasing the STR size, the overall volumetric mass transfer coefficient decreased by at least 20% following a conventional scale-up rule. This was explored by combining the concepts of the local residence time distribution (RTD) of the liquid phase and the local $k_L a$ values inside the STR. These findings revealed the challenges involved in scaling up multiphase stirred tanks. Lastly, some alternative approaches are suggested for the design and scale-up of multiphase reactors that may mitigate the inherent limitations of conventional rules.

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1. Introduction

Gas/liquid stirred tank reactors (STRs) are widely used in the petroleum, chemical, petrochemical, mineral, and metallurgical industries to carry out reactions between gases and liquids. Over the last few decades, the increasing volumes of products manufactured in industrial processes have led to the use of larger and larger reactors. As a result, finding adequate rules for scaling up such processes from the lab to industrial scale has become a crucial task for process engineers.

The design and scale-up of gas/liquid STRs are not straightforward tasks, mainly because chemical reactions are generally related to mass and momentum transfer mechanisms in a complex manner. The current state of the art regarding the scale-up and design of large STRs is based on empirical correlations, best practices (know-how routines), and rules of thumb, even with existing research tools and advances in engineering design. With conventional scale-up procedures, the values of hydrodynamic parameters are assumed to be constant in the entire reactor ("well-mixed" assumption). However, in real cases, especially at the production level, the values of such parameters (the mass transfer coefficient, for example) may vary significantly.

The productivity of many processes is limited by mass transfer between phases, especially in the case of low soluble species in the

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gas phase that transfer to the liquid phase. This includes many bio-processes such as those for the production of expensive specialty chemicals, including proteins, and bulk chemicals such as biofuels, lactic acid, and citric acid, where oxygen transfer is vital for the success of the process [1,2]. Understanding gas/liquid mass transfer is thus essential for the adequate design of mixing systems. The mass transfer rate can be quantitatively defined as the product of the volumetric mass transfer coefficient ($k_L a$) and the driving force, which is the difference between the saturation concentration of gas and its actual concentration in the liquid phase ($C^* - C(t)$). Accordingly, $k_L a$ can affect operations by limiting productivity in various ways, including by changing the rate and, possibly, the selectivity.

The volumetric mass transfer coefficient is very sensitive to the hydrodynamics in the reactor, and predicting the coefficient is extremely difficult due to the complexity of the gas/liquid flows in STRs. Ideally, a uniform $k_L a$ and driving force inside STRs are desirable during scale-up. While there is a distribution of $k_L a$ due to variations in the hydrodynamics governing laboratory-scale STRs, the driving force can still be uniform when the mixing time is much shorter than the mass transfer time scale [3]. However, this is not always true for large STRs, which leads to apparent changes in conversion to lower values, resulting in longer batch or residence times (cyanidation processes, for example) [4] and higher production costs. Moreover, variations in the configuration of the reactor and the physiochemical and rheological properties of the flow may also hinder the transfer capacity of larger-scale STRs.

Numerous correlations have been proposed in the literature that express $k_L a$ as a function of the operating conditions of the STR, including power input per liquid volume (P_g/V_l) and superficial gas velocity (v_{sg}). They were often developed based on experimental data obtained using dynamic methods in laboratory-scale reactors. With this measurement technique, the concentration of dissolved gas over time is measured by a probe, which is calibrated beforehand, and the volumetric mass transfer coefficient is determined from the slope of the natural logarithm of these measured dissolved gas concentrations versus time, employing the least square method and assuming that the STR is “well mixed” [5–8]. The empirical correlations of $k_L a$ are often expressed using the following form:

$$k_L a = C \left(\frac{P_g}{V_l} \right)^a (v_{sg})^b \quad (1)$$

The values of the constants inherent to this correlation that have been proposed by several authors for air/water flows inside an STR agitated by a single Rushton turbine are summarized in Table 1. The table also includes the range of operating conditions in which these parameters were determined. Since the power consumption per liquid volume is a function of the superficial gas velocity, predictions of the $k_L a$ value using these correlations are even more complicated.

The discrepancies in the values of the exponents proposed by various authors can be attributed to differences in the geometries of the systems, the range of operating conditions, and the measurement techniques used. Xie et al. (2014) [13] showed that predictions of these correlations can vary, with standard deviations ranging from 10% to 55%, even without a large difference in the scale of the STR. This means that these correlations are scale-dependent and that their application is limited for the design of large-scale reactors [14–16].

Understanding gas/liquid flow behaviour in terms of operating regimes is vital and should be taken into account for successful STR scale-ups. Yawalkar et al. (2002) [17] used experimental $k_L a$ values drawn from the literature for different sizes of STRs ($T = 0.39$ – 2.7 m) to take the effect of the flow regime into account and proposed the following correlation for $k_L a$ as a function of relative dispersion (N/N_{cd}) (with $\pm 22\%$ accuracy):

$$k_L a = 3.35 (N/N_{cd})^{1.464} (v_{sg}) \quad (2)$$

where N and N_{cd} are the impeller rotational speed and the minimum rotational speed of the impeller for complete dispersion of the gas inside the STR, respectively. Nienow et al. (1977) [18] proposed the following correlation for N_{cd} in STRs equipped with a Rushton turbine:

$$N_{cd} = \frac{4(Q_g)^{0.5} (T)^{0.25}}{D^2} \quad (3)$$

where Q_g , T , and D are the gas flow rate, the tank diameter and the impeller diameter, respectively. Kapic and Heindel (2006) [8] used the same approach and developed the following correlation to predict $k_L a$ of STRs that operate in the effective flow regime:

$$k_L a = 1.59 (N/N_{cd})^{1.342} (v_{sg})^{0.93} (T/D)^{0.415} \quad (4)$$

While these correlations may provide a better prediction for the $k_L a$, at least up to the pilot-scale STRs, they do not provide any information on the local values of this parameter, which brings the concept of imperfect mixing into play.

The effects of imperfect mixing on the performance of reactors have been well characterised by the concept of residence time distribution (RTD) based on the pioneering work by Danckwerts in 1953 [19]. Models based on combinations of well-mixed reactors (compartments) are often used to simulate observed RTD data [20–22]. Relating reactor design, scale, and operating conditions to performance requires many experiments to fit the parameters of the models. Moreover, some concerns still need to be addressed, including the cost of the experimental methods and their scale limitations. Many processes involve high temperatures, high pressures and hazardous conditions for which the acquisition of detailed experimental data is not practical [23].

Thanks to the availability of powerful computers, CFD is being increasingly used to study the effects of hydrodynamics on the performance of reactors. Since it is important to take the local

Table 1
Constants of $k_L a$ correlations (Eq. (1)) for air/water flows inside an STR agitated by a single Rushton turbine.

References	$v_{sg} \times 10^3$ (m/s)	P_g/V_l (W/m ³)	T (m)	C	a	b
Smith et al. (1977) [9]	4–46	20–5000	0.61–1.83	0.010	0.48	0.40
Van't Riet (1979) [5]	5–40	300–3500	0.5	0.026	0.4	0.5
Linek et al. (1987) [6]	2.12–2.42	100–3500	0.29	0.005	0.59	0.4
Hickman (1988) [10]	2–17	50–3500	0.6	0.043	0.4	0.57
			2	0.027	0.59	0.68
Gagnon et al. (1998) [11]	0–1.2	0.001–30	0.23	0.5	0.01	0.86
		30–10,000		12.2	0.57	0.47
Geozork et al. (2001) [12]	0–130	0–100,000	0.29	0.005	0.59	0.27
Zhu et al. (2001) [7]	1–7.5	100–1500	0.39	0.031	0.4	0.5
Kapic and Heindel (2006) [8]	0.5–7.2	–	0.21	0.04	0.47	0.6

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