Characterization of micromixing in a rotor-stator spinning disc reactor: effects of gap distance

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Abstract

In the chemical industry many processes involve complex reaction systems where fast reactions take place, deriving in a range of products while in fact only one is the desired one. In the past, in order to achieve high selectivity and yield towards the main product, a common approach has been to slow down the reactions by diluting the feeding streams, usually with solvents. As a consequence, large reactors are needed to meet the production requirements, and the removal of the solvents derive in high energy costs.

More recently, novel equipment has been developed in the framework of Process Intensification (PI), aiming to enable production conditions that were not possible with traditional equipment by the enhancement of mass and heat transfer rates. With these novel reactors, high yields can be obtained without the need to dilute the reaction systems.

In those high concentrated systems with higher reaction rates, the selectivity is then determined by the mixing efficiency, especially in systems where competitive consecutive or parallel competitive reactions take place. More specifically, for very fast competitive reactions the micromixing time -which is the homogenization of the system at the molecular scale- determines the product distribution. The micromixing time has been extensively investigated and well correlated to the turbulence intensity, mainly in stirred vessels where homogenous and isotropic turbulence is observed.

For novel reactors such as the rotor-stator spinning disc reactor, high shear forces applied to very small reaction volumes lead to a very high turbulence intensity. These are in the range of 4 to 6 orders of magnitude higher than those achieved in stirred vessels. In other words, very high micromixing efficiency is expected[1].

In literature, there are models that can describe the relationship between micromixing time and energy dissipation rate. The micromixing time has been theoretically and experimentally determined to be proportional to the Kolmogorov microscale:

\[ t_{\text{mix}} = C \left( \frac{\nu}{\varepsilon} \right)^{0.5} \] (1)

Where \( \nu \) is the kinematic viscosity of the fluid, \( \varepsilon \) is the (local) energy dissipation rate. One of the most consistent models based on turbulence theory is the Engulfment model[2]. In this model the term \( C \) takes a value of 17.23, based on a derivation from the most hydrodynamic eddy of the turbulent field engulfing liquids from the surroundings and allowing a small reaction zone to
grow and react. Similarly, other models like the incorporation model[3], uses this term C as a correlation to obtain a micromixing time that is proportional to the incorporation of liquids from the surroundings of the reaction zone.

Furthermore, some test reaction systems have been developed, in order to determine the micromixing times[4][3]. Assuming enough knowledge of the kinetics of the system, the fundamental basis of these test reactions is that by performing competitive reactions, one can analyze the product distribution and relate it to a micromixing time, using one of the available models.

In the rotor-stator spinning disc reactors, the shear rate and therefore the energy dissipation rate is known to have a proportionality to the radius of the disc[5][6]:

\[ \varepsilon \propto r^{11/4} \]  \hspace{1cm} (2)

The previous relationship allows for a good estimation of the local energy dissipation rate by performing a momentum balance.

Naturally, by reducing the gap distance between the rotor and the stator, the reactor’s volume will also decrease. This suggests that the energy transferred from the disc into the liquid will be locally higher, and also a function of the gap clearance. In the turbulent regime with merged boundary layers, the shear rate –and energy dissipation rate– is a function of the gap distance [5][6]:

\[ \varepsilon \propto h^{-1/4} \]  \hspace{1cm} (3)

Experimental results in a rotor-stator spinning disc reactor at various gap distances show, however, that there is not significant effect observed when modifying this parameter. In the first graph it can be observed that the estimated local energy dissipation rate obtained from the momentum balance is underestimated for bigger gap distances. On the other hand, on the second graph the results indicate that the main parameter to define the micromixing time is the rotational speeds.

The results suggest that the average local energy dissipation rate estimated from the correlations from literature [6] give a good approximation for the macromixing effects (bubble formation[5], convective heat transfer[7], mass transfer [8]) in the enclosed space between a rotating disc and a wall. However, for the non-homogeneous, anisotropic turbulent field created by the high shear forces in such a small volume, the local energy dissipation rate requires a correlation to the tangential velocity. This is a topic of ongoing research.

Furthermore, a comparison between two test reaction systems is presented, adopting a new kinetic model and addressing previous concerns about the use of the Villermaux-Dushman system (unpublished work). With this new kinetic model, lower micromixing times are obtained than those previously reported using the Villermaux-Dushman method when compared to the Diazo-coupling of naphthols [9]. This is however not surprising, since the iodide-iodate reaction in the Villermaux-Dushman is much faster (kinetic coefficient in the order of magnitude 8) than the diazo coupling of 2-naphthol (kinetic constant in the order of magnitude 5). The iodide-iodate reaction occurs in a more localized zone with higher turbulent intensity.


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