Additions to “Micromixing in a Rotor-Stator Spinning Disc Reactor”

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BACKGROUND

In our earlier publication, we experimentally investigated the micromixing efficiency in a novel type of reactor: the rotor-stator Spinning Disc Reactor (rs-SDR). The Villermaux–Dushman test reaction was chosen because it is relatively simple, in comparison to other test reactions that are sensitive to mixing effects in high-intensity mixers (e.g., the second or the fourth Bourne reaction). Based on the recommendations by Kolb et al., we decided to use perchloric acid as the proton source, instead of sulfuric acid, which is the reagent commonly used in the Villermaux–Dushman protocol. Micromixing times were estimated by means of the incorporation model and compared to the engulfment time, including self-engulfment effects, using the kinetic model from Guichardon et al. However, the validity of the kinetic model using a different proton source was not confirmed, and as noted by other authors, the original kinetic model might only be suitable in combination with sulfuric acid.

In light of the recent publications by Baqueiro et al. and Wenzel et al., which discuss the Villermaux–Dushman method, a decision was made to revise the published results. We investigated the kinetics of the iodide–iodate reaction (the Dushman reaction), using perchloric acid as the proton source. Our preliminary results, presented at the last AIChE Annual Meeting, showed good agreement with other kinetic studies previously published by different authors, even under different experimental conditions. The iodide–iodate reaction is well-described as a fifth-order rate law under the investigated conditions. Furthermore, the effects of ionic strength, which are very important when modeling micromixing using the incorporation model or the engulfment model, show that the dependency of the reaction rate coefficient to the ionic strength can be very well described in a Davies-like equation. Although our first approach for the kinetic study was to fit parameters arbitrarily, it was later concluded that a better explanation of the effects of ionic strength on the activity coefficients of the species can be represented with the model proposed by Bromley.

UPDATED RESULTS AND FURTHER DISCUSSION

Figure 1 shows the updated values of estimated micromixing times, as well as new results obtained with the second Bourne reaction (simultaneous diazocoupling of 1-naphthol and 2-naphthol) under the exact same operational conditions than in our previous publication. This time, the effects of self-engulfment are not considered. It can be seen that the results are very similar, regardless of the test reaction, and are slightly above the well-established engulfment time.

Figure 1. Updated micromixing time as a function of energy dissipation rate, using the E-model but without self-engulfment effects.

Further analysis of these results led to the conclusion that the selected flow rate for the injected acid (10 mL min⁻¹) was leading to mesomixing effects, possibly of turbulent dispersion, which is a topic that is currently investigated in the rs-SDR and requires more experimental work and analysis. Preliminary data indicate that operating with a flow rate of 2 mL min⁻¹ eliminates mesomixing effects, and Figure 2 shows that the estimations of micromixing times, regardless of the test reaction, are in very good agreement with the results of Baldyga and Bourne. In fact, it is observed that the estimation of micromixing times corresponds to the theoretical micromixing time when using the rate of strain of the most active eddy instead of the engulfment rate, where ε is the local energy dissipation rate. As described by Baldyga and Bourne, this can be due to the fact that the engulfment rate typically included a correction for intermittency effects caused by the interactions between macroscopic and microscopic length scales, which is a phenomenon unlikely to occur in the rs-SDR, where the turbulent kinetic energy is generated and dissipated in a very small gap distance of a few millimeters.
The estimated micromixing times reported for the rotor-stator spinning disc reactor are revised. Previously, the Villermaux–Dushman method was applied, using perchloric acid instead of sulfuric acid, to avoid the effects related to the slower second deprotonation, but without validating the kinetic model for the use of a monoprotic acid. An alternative kinetic model is now employed, and it is suggested for the use of monoprotic acids.

In addition, a closer look at the results showed mesomixing effects in our previous publication, which are now avoided by reducing the injection flow rate of the acid. A comparison of estimated micromixing times obtained with the second Bourne reaction and the Villermaux–Dushman method shows that they are in very good agreement with the theoretical lifetime of the most active eddy in a turbulent field.

This alternative kinetic model does not invalidate other results obtained with sulfuric acid, but it can be a better option to obtain higher sensitivity toward mixing effects and avoid the discussion of the incomplete dissociation of the sulfuric acid.

Until direct numerical simulations are available to resolve the complex hydrodynamics of the rs-SDR, we will continue to investigate micromixing (and mesomixing) effects, using the incorporation model, together with test reactions.

# FINAL REMARKS

The estimated micromixing times reported for the rotor-stator spinning disc reactor are revised. Previously, the Villermaux–Dushman method was applied, using perchloric acid instead of sulfuric acid, to avoid the effects related to the slower second deprotonation, but without validating the kinetic model for the use of a monoprotic acid. An alternative kinetic model is now employed, and it is suggested for the use of monoprotic acids.

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# ASSOCIATED CONTENT

*Supporting Information*

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.iecr.0c03157.

Theoretical background, including a summary of the derivation regarding the “most active eddy” in the turbulent field from Baldyga and Bourne, and reflections (PDF)

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**Notes**

The authors declare no competing financial interest.

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