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A New Mixing Diagnostic: Mixing Sensitive Chemistry with Phase Change

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Abstract

Mixing-sensitive competitive reactions with phase change are known to occur in industrial reactors. In particular, we are interested in the evolution of a gas phase from liquid reactants. Examples include when a volatile product forms directly from the reaction, or when rapid pressure drop and temperature rise in the mixing zone causes reactants or products to form a gas phase. There has been significant literature on the mixing sensitive chemistry in single phase system. Prud'homme and Johnson (2003) investigated the micromixing present in a confined impinging jets (CIJ) mixer by proposing a "chemical ruler" for the second-order competitive reaction set, to assign an absolute value to the mixing time in the CIJ mixer. Their analysis showed that the characteristic mixing time in a CIJ mixer scales as the inverse of jet velocity to the three halves power. However, the present analysis showed that the similar analogy can not be used to address the micromixing in the system with phase change.

To address the micromixing present in the mixing sensitive chemistry with the phase change, a similar CIJ mixer system is used with jet diameters of 1 mm and 3 mm. The second order competitive reaction set, involving acid (hydrochloric acid) and base (sodium bicarbonate) neutralization in parallel with di-methoxy propane (DMP) hydrolysis, is used to induce flashing in the system. The hydrolysis reaction competes for acid with the "instantaneous" neutralization. As $NaHCO_3$ is rapidly neutralized with HCl, gaseous CO_2 evolves from the reaction mixture.

The chemistry was tested in a small impinging jet reactor. Results have shown that the technique is promising; the gas evolves rapidly enough to impact the reaction selectivity. For the impinging jet, visualization experiments showed that the gas evolution was visible in the mixing zone. Hydrolysis increased dramatically over the non-gassed case. This is attributed to the impact on the micromixing as the gas formed a barrier between the impinging flows. The overall flow pattern is altered as well. In contrast to the single phase mixing, the mixing time in the phase change system is not only a function of jet velocity and turbulent energy dissipation but also on the effect of phase change on the localized turbulent dissipation rate and local flow structure. The conventional Damkohler number can not be used to correlate the processing. This analysis also calls for further investigation in deriving the mixing time correlation as a function of phase change, towards predicting the mixing performance, reaction selectivity, and scale-up criteria.