

346a Application of Computational Fluid Dynamics in Liquid Reactions

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In many industrial applications, liquid reactions are used to convert raw material into desirable products. Mixing is well known to have a great impact on product selectivity in reactors. For instance, in parallel or competitive-consecutive reactions, final product distribution is not only dependent of the reaction kinetics, but also of the way how reagents are mixed down to the molecular level where reactions actually happens. Computational Fluid Dynamics (CFD) has been increasingly used to represent, design and scale-up mixing processes in industry. In order to accurately predict interactions between reaction and mixing, besides macro-mixing and meso-mixing, micro-mixing needs to be accounted for as well. Many numerical methods are available for micro-mixing predictions. Each method has its advantages and disadvantages. In this presentation, several such methods including the composition pdf, the constructed pdf, the DQMOM-IEM and the eddy dissipation concept model will be reviewed, and their application in the simulation of a confined impinging jet reactor will be discussed. Results from different numerical methods will be compared with the experimental data reported by Johnson & Prud'homme. Numerical cost and accuracy of each method will be assessed.