133c Modeling Competitive Liquid Reactions

Genong Li, Ying Liu, Graham Goldin, Rodney O. Fox, and Kumar Dhanasekharan Mixing at a molecular scale, commonly referred to as micromixing is well known to have a great impact on product selectivity in liquid reactions used in the pharmaceutical industry. 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, micromixing needs to be accounted for in the modeling. Many numerical methods are available for micromixing predictions with CFD. In this presentation, the simulation of a confined impinging jet reactor will be discussed and the product selectivity will be compared with the experimental data reported by Johnson & Prud'homme.