

466d Understanding Selectivity of an Exothermic Lithiation Reaction in a Semi-Batch Reactor Using CFD and Kinetic Modeling Tools

David J. Am Ende, Eric L. Dias, and Jason Mustakis

In the development of a lithiation of dibromobenzene in a synthetic process we observed a significant mixing dependence on selectivity. The reaction is highly exothermic and so heat transfer and mixing were both found to be important in maintaining selectivity. To further understand the mechanism controlling selectivity, mechanisms were proposed and supported by a kinetic analysis performed under using BatchCad to estimate reacton rate constants at several temperatures. CFD (Fluent) was used to gain insight into localized temperature gradients (hot spots) within the reactor and especially near the n-butyl lithium feed point. A summary of the calorimetry, FTIR data, kinetic analysis, and CFD modeling will be presented.