133a Predictive Kinetic and Reactor Modeling Using Aspentech Batchcad

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Process modeling using software such as BatchCAD has been conducted by our group over the last few years to complement inline monitoring and reaction calorimetry. This talk reviews several recent applications of predictive modeling as a tool for building the detailed understanding necessary for safe and efficient process development, including two current case studies. Kinetic studies of a coupling reaction using inline FTIR have been used to develop a model of product and impurity formation. This model can then be used to aid in a mechanistic understanding of the process and assist in analyzing process robustness. Infrared and calorimetric studies have also been used to develop a kinetic model for improved understanding of another coupling reaction.