

“Modeling and Optimizing Adiabatic Multiphase, Multisolid Reaction Systems with DynoChem”

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Abstract:

A reaction step in a Monsanto intermediate chemical process had been developed in 1999 by a Monsanto Fellow in R&D - Dr Robert Weisenfeld. Dr Weisenfeld used ACSL (Advanced Control Simulation Language) as the programming platform for this model, and developed the complete set of differential balances and rate expressions for phase transports from first principles. The reaction step contains many complex and interactive phenomena – aqueous ionic reactions, phase dissolution of one component and crystallization of another, adiabatic temperature rise and exothermic heat removal through vaporization, and temperature reduction through depressurization. He developed and used a combination of data from fundamental laboratory reaction / crystallization / dissolution experiments, and plant operation to fit the constants required with the fitting routines from this ACSL software. The code in ACSL consisted of 26 pages of 8^{1/2} x 11 inches.

This model was used extensively after development to define optimum operating conditions for the plant while maximizing production rate and yield. During the last 6 years, the plant operations have evolved to achieve ever higher production rates, so a need was identified last year to define a new window of optimum yield operations while maximizing production rate. DynoChem was chosen as the test platform to transform the ACSL code into a new simulation environment to enable easier access to the optimization module.

The presentation will focus on how some of the shortcomings from ACSL were overcome by DynoChem, and what steps were taken to prepare the model for use in optimization by plant operations people.