

Purdue Parallel Modeling System (PPMS): Cyber-Infrastructure for Kinetic Model Development

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The development of quantitative models to describe the reaction kinetics for complex chemical reactions needs tools to (i) rapidly development the appropriate differential/algebraic equations associated with a complex set of chemical reactions and (ii) fit kinetic parameters and critically evaluate/revise a postulated kinetic mechanism with respect to experimental data. The development of the appropriate differential-algebraic equations (DAEs) can be a daunting task for a number of important chemical systems where the number of species can exceed 1000 and the number of binary reactions can exceed 10^6 (e.g. polymerization, sulfur vulcanization of rubber, hydrocarbon cracking/reforming, etc.). Parameter determination by traditional optimization methods is computationally intense for such large systems. Moreover, the equations are inherently nonlinear due to binary reactions and Arrhenian (i.e. exponential temperature dependence), where nonlinear Bayesian methods are needed vs. traditional linear least squares; however, Bayesian tools are not conveniently available to chemical researchers and computationally very intense.

In order to address these issues we have developed a suite of cyber-enabled tools that we have called the Purdue Parallel Modeling System (PPMS). The PPMS includes (i) several chemical compilers that allow the researcher to postulate the chemical mechanism in a series of near-English language, where the compilers then automatically generate the appropriate rate expressions and associated DAEs, (ii) a MatLab-like interface for simple DEA sets of kinetic equations that generates the associated C++ code, (iii) a parallelized Levenberg-Marquardt code that enables fitting of multiple data sets (iv) a suite of parallelized nonlinear Bayesian codes for parameter estimation including uncertainty, model evaluation and model discrimination and (v) work is underway on an automatic connection with graphical output. The parallelized Levenberg-Marquardt and Bayesian codes have all been enabled to run on the TeraGrid, allowing the chemical researcher access to the necessary computational resources without unnecessary IT overhead. The PPMS will be demonstrated on a series of problems, including (i) olefin polymerization by single-site Group IV catalysts, (ii) sulfur vulcanization of rubber and (iii) epoxy cure kinetics.