

PrIME - Process Informatics for Chemical Reaction Systems

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Right now, the branch of chemical kinetics is transforming from a "post-dictive" field that reproduces experimental results to one that predictively models complex systems and tells researchers what to expect in their experiments, saving substantial amounts of time and money.

Constructing accurate kinetic models requires several factors. Among the most important are: (1) A chemical mechanism that properly describes the system of interest. (2) Reliable experimental rate constants to parameterize the model, (3) a fast means for estimating the unknown rate constants, and (4) methods to gauge the overall error in the model due to errors in the parameters (both experimental and theoretical). The PrIME project is a massive, collaborative project spanning many research groups in top universities and laboratories (MIT, U.C. Berkeley, Stanford, the National Institute of Standards, etc.) that seeks to address all of these factors in gas phase kinetics.

The approach is multi-faceted: The Green group's reaction mechanism generation (RMG) software will be incorporated to generate the reaction models. Experimental data will be centralized and evaluated for reliability into a massive database so that they can be used in the models automatically. The system will enable experimentalists to submit their experimental data via the Internet, both as final results and in a raw form. The raw data will enable the system to assess the inherent errors and to compare measurements from different experiments. The models constructed will be able to take into account the reliability of different measurements to make error estimates in the model. Eventually, it should be able to make recommendations as to which parameters need to be improved (via new experiments or better theoretical calculations) in order to reduce the estimated error by a user-specified amount. Furthermore, by standardizing the way chemical kinetics models are made and used, PrIME hopes to improve the quality and reproducibility of model predictions overall. Though much of the basic infrastructure is already in development, there remains much work to be done in order to bring this project to fruition.