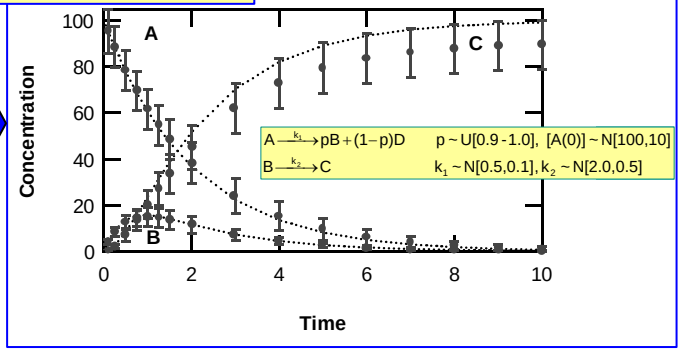
$$E[y(\boldsymbol{\theta})] = \int_y y(\boldsymbol{\theta})\, f_{y(\boldsymbol{\theta})}\, dy(\boldsymbol{\theta}) \equiv \int_{\boldsymbol{\theta}} \cdots \int y(\boldsymbol{\theta})\, f_{\boldsymbol{\theta}}\, d\theta_1 \cdots d\theta_m$$

Calculation of the effects of parameter uncertainties on the predictions of a kinetics model.



Chemical Libraries, Uncertainties

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Abstract

When mathematical models are used to describe chemical kinetics problems there are inevitable uncertainties in the experimental determinations of reaction rate constants, measurements of initial conditions or in the species concentration profiles. The fact that there are uncertainties is not the issue – they are always present. The challenge is to identify those that contribute most to uncertainties in predicted outcomes and then, in turn, use this information to refine the measurement programs or the parameterization of the kinetic models themselves. This presentation will describe work underway as part of the NSF sponsored PrIME[1] (Process Informatics Model) project to develop ways to represent uncertainties in the information data bases so that the representations are compatible with emerging computational algorithms that predict the probability density functions of the outputs from kinetic models. Particular emphasis will be given to the use of XML schema as a way to represent descriptions of parameter uncertainties. A key objective of the research is to help the institution of more systematic ways to collect data about parameter uncertainties and represent this information in modern relational data base systems. Several illustrative example will be used to illustrate the concepts an show how the uncertainty descriptions can be used in Monte Carlo, Latin Hypercube and Polynomial Chaos based algorithms for uncertainty propagation.

[1] The PrIME project is described in more detail in the presentation by M. Frenklach.