Quantification of the Uncertainty of Parameters in Chemical Kinetics

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Many models in science and engineering use chemical kinetics parameters and thermodynamic data. The accuracy of simulation results and the predictive power of these models rely on the precision and level of uncertainty of the chemical kinetics and thermodynamic parameters. Several methods exist for the quantification of the uncertainty of these parameters:

(i) If the parameter is the direct result of a measurement, then the uncertainty of the measured data have to be estimated.

(ii) The parameter (*e.g.* rate coefficient at a given temperature and pressure, or the standard enthalpy of formation of a species) can be the result of a theoretical calculation. The accuracy of such calculations depends on the level of theory and the accuracy of the data used.

(iii) Optimization of chemical kinetic models or thermodynamic networks leads not only to well established parameters, but also a quantification of the uncertainty of the fitted parameters. Following the pioneering work of Michael Frenklach et al. [1], [2] and Branko Ruscic et al. [3] in chemical kinetics and thermodynamics, respectively, several groups developed the optimization methodology in both fields.

In the lecture the main features of the quantification of the uncertainty of rate parameters will be reviewed and the approach developed in our group will be presented.

[1] Frenklach, M. *Combust. Flame*, 58:69–72, 1984.
[2] Frenklach, M., Wang, H., Rabinowitz, M.J. *Prog Energy Combust Sci*, 18:47–73, 1992.
[3] Ruscic, B., Pinzon, R.E., Morton, M.L., von Laszewski, G., Bittner, S., Nijsure, S. G., Amin, K. A., Minkoff, M., Wagner, A. F. *J. Phys. Chem. A* 108:9979–9997, 2004.