BASIC ENERGY SCIENCES
BES SEMINAR SERIES

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10:00 A.M. Seminar | Room 209

"Optimization of rate parameters of detailed reaction mechanisms"

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Abstract

Chemical kinetic measurements can be either direct or indirect. In direct measurements, the reaction conditions are selected in such a way that the measured signal depends mainly on the rate coefficient of a single reaction step. In the indirect measurements (*e.g.* ignition time or laminar flame velocity measurements), the measured signal depends on the rate parameters of several elementary reactions and the data can be interpreted via simulations using a detailed reaction mechanism. Determination of rate parameters of gas phase elementary reactions is usually based on direct measurements. The rate parameters obtained in many independent direct measurements are then checked by doing ignition or flame simulations. Using this approach, the uncertainty information for the rate parameters is based on the direct measurements only and this uncertainty is usually rather large.

A new approach has been suggested that takes into account both direct and indirect measurements. First, the domain of feasibility of the rate parameters (Arrhenius parameters, third body efficiencies, parameters of temperature dependence *etc.*) of several selected reaction steps is determined from all available direct measurements. Then, the optimal rate parameters are searched for within this domain to reproduce the several thousand selected direct and indirect measurements. A new global fitting algorithm was developed which also provides information about the covariance matrix of all rate parameters. Application of the method significantly decreased the uncertainty of the rate parameters of the investigated reaction steps and provided information about their correlation.

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