Sensitivity Analysis in Chemical Kinetics

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The Fifth International Conference on Sensitivity Analysis of Model Output (SAMO 2007) was held from 18 to 22 June 2007 at the Eötvös University (ELTE), Budapest, Hungary. The conference was jointly organized by the Institute of Chemistry of ELTE and the IPSC section of the European Commission Joint Research Centre (Ispra, Italy). The previous SAMO conferences were held in Belgirate, Italy (1995); Venice, Italy (1998); Madrid, Spain (2001); and Santa Fe, NM (2004). Sensitivity analysis investigates how a model depends on its input parameters. SAMO is a series of conferences devoted to the development and applications of sensitivity analysis methods. These methods are widely used in chemistry, physics, biology, engineering, environmental science, nuclear and industrial safety, and economics.

At the SAMO 2007 conference, there were 81 participants from 21 countries. The participants presented 8 invited lectures, 28 lectures, and 43 posters. The abstracts of all presented works and the slides of most lectures are available at the conference Web site: http://samo2007.chem.elte.hu/

Chemical kinetics is very closely linked to sensitivity analysis. At the evaluation of kinetic experiments, rate parameters are frequently determined via nonlinear parameter estimation. Sensitivity analysis can be used to identify the influential parameters and to pinpoint the cases when only the ratio or product of the parameters can be determined. In a similar way, sensitivity analysis can be used for experimental design that is to determine the conditions and setup of experiments that provide the most information from a series of measurements. Critical compilations of rate parameters list not only the recommended kinetic parameters but also report the accuracy of the data by assigning an uncertainty factor to them. Uncertainty analysis of models that employ detailed reaction mechanisms can be carried out using these uncertainty factors. The increasing knowledge on the kinetics of many reaction systems is reflected in the increasing size of detailed reaction mechanisms. Sensitivity analysis can be used to identify the redundant species and reactions and thus allows mechanism reduction. These reduced mechanisms can provide almost identical concentration profiles for the important species. Because of the high importance of sensitivity analysis in chemical kinetics, all major simulation codes offer local sensitivity analysis as an option. In accordance with the continuously increasing capacity of computers, it is expected that several methods of global sensitivity analysis will appear soon in the simulation codes.

This special issue contains the following seven works that were originally presented at the SAMO 2007 conference:

1. E. Borgonovo, S. Tarantola: Moment independent and variance-based sensitivity analysis with correlations: An application to the stability of a chemical reactor
2. N. Carrasco, S. Plessis, P. Pernot, M. Dobrijevic: Toward a reduction of the bimolecular reaction model for Titan's ionosphere
3. A. Lovrics, I. Gy. Zsély, A. Csikász-Nagy, J. Zádor, T. Turányi, B. Novák: Analysis of a budding yeast cell cycle model using the shapes of local sensitivity functions

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4. J. C. Prince, C. Treviño, F. A. Williams: Reduced kinetic mechanism for high-temperature propane ignition
5. H. Yue, M. Brown, F. He, J. Jia, D. B. Kell: Sensitivity analysis and robust experimental design of a signal transduction pathway system
6. T. Ziehn, A.S. Tomlin: A global sensitivity study of sulfur chemistry in a premixed methane flame model using HDMR
7. I. Gy. Zsély, J. Zádor, T. Turányi: Uncertainty analysis of NO production during methane combustion

These papers are few in number, but represent all major areas of applications of sensitivity analysis in chemical kinetics, such as combustion chemistry (Prince et al., Ziehn and Tomlin, Zsély et al.), atmospheric chemistry (Carrasco et al.), reactor theory (Borgonovo and Tarantola), and biochemical kinetics (Lovrics et al., Yue et al.). The topics of these works include experimental design (Yue et al.), mechanism reduction (Carrasco et al., Prince et al.), uncertainty analysis (Ziehn and Tomlin, Zsély et al.), and model analysis (Lovrics et al.).

Two of the papers contain methodical novelties that may soon become important in chemical kinetics. In the near future, more information will be available about the correlation of rate parameters and thermodynamic data. The paper of Borgonovo and Tarantola discusses moment independent sensitivity analysis considering correlations. The high dimensional model representation (HDMR) method (Ziehn and Tomlin) is able to express the input–output relationship of a complex model with a high dimensional input space. This way a fully functional surrogate model can be constructed with low computational effort, which may become a useful tool in several areas of chemical kinetics modeling.

It is expected that the chemical kinetics community will remain a heavy user of the mature and the newly developed methods of sensitivity analysis.