UNH Materials Science Seminar

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DeMeritt Hall 209B
University of New Hampshire

A 21st Century Approach to Chemical Kinetics

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A major goal of chemical kinetics is to develop computer models detailed enough and accurate enough to assist in design of new processes and materials. This is a very challenging problem for several reasons, even for relatively well-characterized systems:

1) it is hard to construct and solve reacting flow simulations involving complex chemistry, both because the chemistry is very complicated and because there are very serious numerical issues. These challenges are particularly serious for multi-phase systems and for systems where the fundamental thermochemistry is not well understood (e.g. most systems involving metal atoms.)

2) it is very difficult to refine these models using experimental data – seldom is there a single unique model consistent with all the available experimental data, uncertainties are hard to quantify, and it is hard to identify and use all the relevant experimental data.

3) it is hard to document, much less test, all the assumptions and approximations made in steps 1 & 2 - so typically no one knows why two models disagree with each other or with experiment, nor what should be done to improve the situation.

Despite all these challenges, it is now becoming possible to construct predictive chemical kinetic models suitable for design applications, and to qualitatively improve the way kinetics research is done by the community. A vision for the future, and some practical steps already being taken, will be outlined.

After receiving his Ph.D. in experimental Physical Chemistry from Berkeley in 1988, Dr. Green received Postdoctoral Fellowships from both the NSF and NATO to study Theoretical Chemistry at Cambridge University. While in Cambridge, he was named The Charles & Katherine Darwin Research Fellow by Darwin College. In 1991 he joined Exxon Research & Engineering, where he studied the free radical chemistry of fuels, lubricants, and antioxidants both theoretically and experimentally. In 1997 Prof. Green joined the Chemical Engineering faculty at MIT. His research focuses on developing reliable methods for predictive modeling of complex reaction kinetics, including quantum rate calculations and methods for modeling reacting flows. Prof. Green has published more than 80 articles in refereed journals. He is an Associate Editor of the *International Journal of Chemical Kinetics*. He received the NSF CAREER award in 1999. In 2004 he received the American Chemical Society (ACS) Glenn Award in Fuel Chemistry, and in 2005 he received the ACS Certificate of Merit in Environmental Chemistry.