Extending Reaction Mechanism Generator (RMG) to Novel Chemical Systems*

Belinda L. Slakman
Department of Chemical Engineering
Northeastern University
Boston, MA 02115

Reaction Mechanism Generator (RMG) is a software package used to automatically build detailed kinetic models for gas-phase combustion. Other chemical systems with many reaction paths could benefit from this approach. To enable liquid-phase mechanism generation, solvation corrections to reaction rates were found using quantum chemistry and generalized into trends. These trends will allow RMG to automatically predict similar reaction rates.

Functionality was added to RMG to generate models for silicon-based CVD, including published mechanisms, new reaction families, and calculated thermodynamics. Comparison of an RMG-generated model for SiH_4 CVD to published results proves the concept, with suggestions for model improvement presented.

*This work was supervised by Professor Richard West, Department of Chemical Engineering, Northeastern University, Boston, MA and Harsono Simka, Intel Corporation, Santa Clara, CA.