Using Reaction Mechanism Generator (RMG) to study complex liquid-phase systems

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

Liquid-phase chemical systems are important for a variety of applications involving the petrochemical industry, environmental concerns, and human health. However, these reaction systems of interest can be extremely complex. For example, the reactions involved in secondary aerosol formation can contain hundreds to thousands of chemical species, and mechanisms of antioxidants in the body include synergistic effects as well as consideration of many reactive oxygen species. Elucidating the thermodynamic and kinetic parameters of these reaction systems manually is tedious; therefore, we turn to automatic mechanism generation. Specifically, the Reaction Mechanism Generator (RMG) is an open-source software tool for predicting kinetic models of large reaction networks, and uses a flux-based approach to limit the size of these models. RMG works well for combustion systems in the gas-phase, but modifications must be made for liquid-phase systems.

Thermodynamic corrections for liquid-phase systems have been previously incorporated into the Java version of RMG (RMG-Java) using linear solvation energy relationships and a group additivity approach. To account for diffusion limitations on bimolecular reactions, the Stokes-Einstein equation is used. These existing solvation corrections will be added into the Python version of RMG (RMG-Py). Family-based, intrinsic kinetic solvent corrections into RMG-Py will also be added by investigating reactant and transition state energies using quantum chemistry

methods. Finally, the improved program will be used to investigate the effect of an antioxidant on combatting lipid peroxidation in the human body, a model liquid-phase system.