Automated kinetic parameter calculation via transition state theory for bimolecular reactions to develop a 2,5-dimethylfuran combustion mechanism

Pierre Bhoorasingh
Department of Chemical Engineering
Northeastern University
Boston, MA 02115, USA

Increasing energy demands and environmental concerns motivate the development of sustainable energy technologies, with liquid biofuels expected to be the major source of transportation fuels. 2,5-dimethylfuran has been proposed as a possible alternative liquid fuel and can be produced from waste biomass feedstocks, but its combustion properties are poorly understood. A detailed kinetic model would provide insight to the key pathways involved in the fuel combustion and pollutant formation. However, detailed kinetic models are often large, so manual construction of these mechanisms is laborious and error prone. As a result, automatic network generators have been developed to apply chemical knowledge in building these complex reaction networks. Such mechanisms require a high number of kinetic parameters to properly describe the reaction system, but many of these rates are estimated since they are unknown. As these estimates are often very approximate, an on-the-fly method to calculate the kinetic parameters via transition state theory is desired to improve model accuracy.

Distance geometry will be used to create 3-dimensional molecular structures required for external computational chemistry programs to search, optimize, and validate transition state geometries. The optimized geometries will be used to

calculate transition state and reactant molecular properties required for rate calculation via transition state theory. These methods will form an on-the-fly kinetic calculator, which will be tested by developing a detailed 2,5-dimethylfuran combustion model.