541b A Systematic Approach for Automated Reaction Network Generation

Shuo-Huan Hsu, Balachandra B. Krishnamurthy, Prathima Rao, Chunhua Zhao, Suresh Jagannathan, and Venkat Venkatasubramanian

Chemical reaction networks play an important role in the design of chemical processes, discovery of novel materials and so on. However, due to their complexity, the generation, manipulation and management of such networks continues to remain as an ad hoc activity which would benefit from automation in a systematic manner. Only after the reaction network structure is generated, the kinetic parameters can then be determined based on the experimental data and the reaction mechanism is verified.

In this work, we propose a knowledge-based system towards that goal. Ontology[1], which is a set of explicit formal specifications of the terms in a particular domain, has been created for chemical species and reaction mechanisms, including the characteristics of different types of atoms, bonds, molecules, and reactions. The ontologies are the foundation of this system. Ontology enables sharing common understanding of the information among people or software agents; reusing domain knowledge, making domain assumptions explicit, and separating domain knowledge from the operational knowledge. The ontologies are encoded in the Web Ontological Language (OWL) [2]. OWL is based on the description logic, and therefore the system can classify molecules or fragments to predefined molecular patterns and check the semantic consistency between these individuals. The reaction mechanisms are modeled as set of individuals of the defined ontology. An execution engine has been developed to use the reaction mechanisms and molecules to generate reaction network. It can also verify the correctness and consistency of the results. Through the graphical interface, user can construct his/her own chemical reaction knowledge, and visualize molecules as well as the reaction networks.

The ultimate goal of this work is to build a software tool that the chemist can compose a new reaction network efficiently using the chemical knowledge stored in the system. The possibility of using the system to suggest possible reactants and associated reaction mechanisms, given the desired target products and a list of reactant candidates, is also investigated. Combined with parameter estimation techniques, the system can also be used as a hypothesis generator which is very important for kinetic modeling.

Reference

[1] N. Noy and D. L. McGuinness, "Ontology Development 101: A Guide to Creating Your First Ontology", Stanford University, Report SMI-2001-0880, 2001.

[2] D. L. McGuinness and F. van Harmelen, "OWL Web Ontology Language Overview", W3C Recommendation, 2004.