Kinetic Modeling of Syngas Production From Bio-Oil Gasification

Fariba Seyedzadeh
Department of Chemical Engineering
Northeastern University
Boston, Massachusetts 02115

Global warming due to greenhouse gas emissions, increasing energy demands, and decreasing fossil fuel resources have increased interest in renewable fuels made from biomass. The major products of biomass fast pyrolysis under high temperature and pressure are liquid bio-oil, hydrogen, carbon monoxide, carbon dioxide, light hydrocarbons, and solid bio-char. Bio-oil has the potential to be used directly as a fuel, or converted to syngas. Syngas from bio-oil gasification is a valuable chemical mixture and mainly contains carbon monoxide, carbon dioxide, hydrogen and methane. Expensive transportation of biomass as a low density but bulky and polluting material, and problematic direct conversion of biomass to syngas, makes processing via a bio-oil intermediate appealing: bio-oil, a high-density liquid, is easily transportable. The major components of bio-oil are acids, ketones, aldehydes, alcohols, and furans derived from cellulose and hemicellulose, and phenolic and cyclic oxygenates derived from lignin.

The efficiency of bio-oil conversion to syngas is highly dependent on operation conditions of the process. Optimization of process conditions requires an improved understanding of the chemical kinetics of thermal cracking reactions involved in bio-oil gasification. Usually the number of the species and reactions involved in detailed kinetic models are very large. As manually calculating all the model parameters is impossible, the only reliable way to build large detailed kinetic models is on a computer. In recent years several computational algorithms to build large kinetic models have been developed.

In this work we develop detailed kinetic models for bio-oil gasification using Reaction Mechanism Generator software, RMG. The detailed kinetic models are imported to Cantera, an open source software package for modeling chemical kinetics, thermodynamics, and transport processes, and also used to determine the characteristics of bio-oil gasification in batch and CSTR reactors under different operating conditions. The effects of RMG parameters on the model predictions are investigated, as well as the influences of pyrolysis temperature, residence time, and pressure on the syngas yields. The ratios of major gaseous products are compared with experimental works and finally the operation conditions are optimized to maximize syngas yield according to the model.