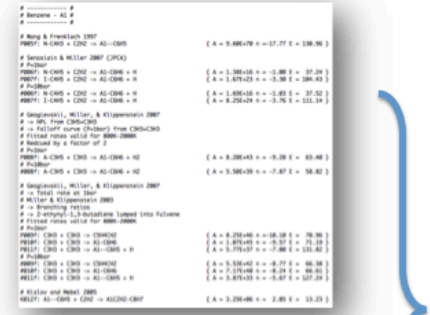
M.Eng./ Undergraduate Research Projects

A Graphical User Interface for the systematic analysis of pollutant formation pathways during biofuel combustion

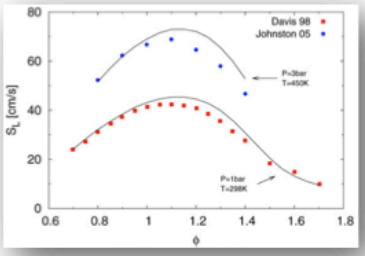
There is an increasing interest in finding reliable and renewable sources of liquid transportation fuels to displace part of our fossil fuel consumption. However, most bio-fuels have a chemical structure and composition quite different from conventional, petroleum-based fuels. These differences, in turn, introduce significant changes in the combustion processes, which affect both the efficiency and emissions of engines. A procedure known as reaction pathways analysis can be used to identify the major chemical routes for fuel decomposition, heat release, and products formation, thereby allowing to better understand and quantify the differences between fossil fuels and biofuels. However, the analysis becomes extremely tedious, if not impossible, when applied to recently developed biofuel combustion models, which commonly involve thousands of species and tens of thousands of reactions.

Project objectives: Facilitate the analysis and comparison of various liquid fuel combustion characteristics through the development of an automated diagnostic tool providing a visual summary of the most important chemical pathways involved in the combustion of a given fuel.

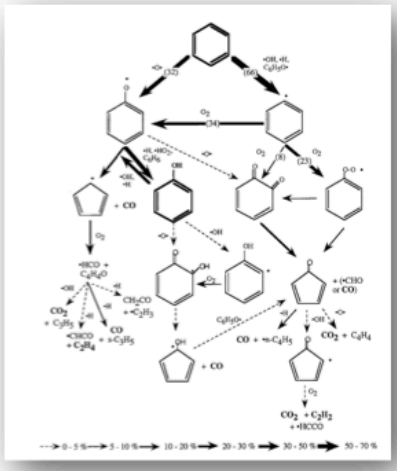
Keywords: GUI development, graph analysis, chemical kinetics, biofuels



Kinetic model for hydrocarbon oxidation



Simulated combustion characteristics



Reaction pathways analysis
(reproduced from Da Costa et al., IJCK, 2003)

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