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Master Thesis Defense

Title

A COMPUTATIONAL INVESTIGATION INTO THERMO-KINETIC PARAMETERS GOVERNING THE DECOMPOSITION OF BIO-OIL MODEL COMPOUNDS

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Abstract

Among notable products from thermal degradation of biomass are simple oxygen-containing aromatics. These compounds typically appear in high loads in collected bio-oil derived from biomass. As such, it is important to comprehend the decomposition chemistry of this category of compounds. This thesis takes on board a general approach to report thermo-kinetic parameters that govern decomposition of a selected set of bio-oil model compounds in two distinct systems: firstly radical-derived pathways in the gas phase and secondly thermal degradation in their condensed media. The first is attained through accurate density functional calculations while the second is accomplished through the use of Model-free and model-fitting approaches to analyse mass loss curves attained in thermogravimetric analysis (TGA). In the first part of thesis, we explored reactions of the hydroperoxyl (HO2) radicals' anisole, cresol, guaiacol, and vanillin with the underlying aim to assess the accuracy of existing kinetic models in the literature in predicting their ignition delay time; an important combustion character of a fuel. Using updated kinetic parameters for initial H abstraction reactions by HO2 from these bio-oil model compounds has only slightly altered ignition delay times while considering various operating pressures. Along the same line of enquiry, we found that radical-derived decomposition of cresol and guaiacol to take place predominantly through abstraction of the hydroxyl'H with a noticeable contribution for abstraction from the methyl site. In case of vanillin, abstraction from the aldehyde's and hydroxyl'H assume comparable importance. We calculated bond dissociation enthalpies in these compounds as to locate the preferable abstractable sites. Arrhenius parameters were provided for a large set of reactions. Such findings are expected to enhance the accuracy and predictability of kinetics models that account for oxidative and pyrolytic decomposition of biomass surrogate compounds. In attaining the second objective of the thesis and based on the obtained TGA and DTG profiles, model-free methods, specifically the KAS model, FWO model, and Starink model were used to derive thermo-kinetic parameters for oxidative and pyrolytic decomposition of for catechol and maltol. Decomposition mechanisms were then determined using the Coats and Redfern method for fitting kinetics. It is hoped that outcomes of this work to advance our comprehensions of the complex chemical reactions that prevail during decay of bio-oil model compounds.

Keywords: Bio-oil model compounds, DFT, Radicals, TGA, Arrhenius parameters, Mechanisms, Kinetics, Radicals.