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Computational Fluid Dynamics Modeling of Liquefaction of Wood and It's Model Components Using a Modified Multistage Shrinking-Core Model

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Abstract : Wood degradation in hot compressed water is modeled with a Computational Fluid Dynamics (CFD) code using cellulose, xylan, and lignin as model compounds. Model compounds are reacted under catalyst-free conditions in a temperature range from 250 to 370 °C. Using a simplified reaction scheme where water soluble products, methanol soluble products, char like compounds and gas are generated through intermediates with each model compound. A modified multistage shrinking core model is developed to simulate particle degradation. In the modified shrinking core model, each model compound is hydrolyzed in separate stages. Cellulose is decomposed to glucose/oligomers before producing degradation products. Xylan is decomposed through xylose and then to degradation products where lignin is decomposed into soluble products before producing the total guaiacol, organic carbon (TOC) and then char and gas. Hydrolysis of each model compound is used as the main reaction of the process. Diffusion of water monomers to the particle surface to initiate hydrolysis and dissolution of the products in water is given importance during the modeling process. In the developed model the temperature variation depends on the Arrhenius relationship. Kinetic parameters from the literature are used for the mathematical model. Meanwhile, limited initial fast reaction kinetic data limit the development of more accurate CFD models. Liquefaction results of the CFD model are analyzed and validated using the experimental data available in the literature where it shows reasonable agreement.

Keywords : computational fluid dynamics, liquefaction, shrinking-core, wood
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