A SURROGATE MODEL CONSTRUCTION STRATEGY FOR BIO-OIL USING ReaxFF MOLECULAR DYNAMICS

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Surrogate fuel model is useful as representative of simplified complex fuel mixture in description of their chemical kinetics in pyrolysis or oxidation conditions. This work propose a surrogate model construction strategy for bio-oil using ReaxFF molecular dynamics. A 24-component bio-oil model was constructed as a baseline model for real bio-oil based on the literature reported data of GC-MS analysis for bio-oil yielded from fast pyrolysis of *Pterocarpus Indicus*. According to the chemical constituent and functional groups in the 24-component bio-oil model, 5 surrogate bio-oil models each containing 6 components were formulated. ReaxFF MD simulations are performed on the 6-component surrogates and the 24-component oil model under the same oxidation conditions. In addition to element ratio comparison, the surrogate models are validated by comparing the simulated temporal evolution of major reactants and products including radicals using the 24-component model as a baseline.

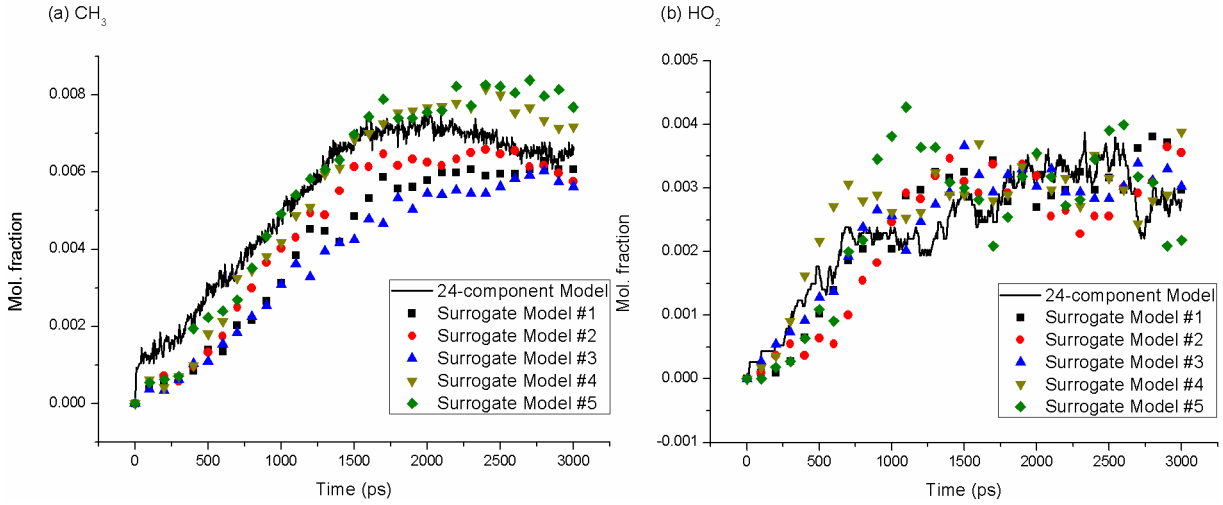

Figure 1 – Time evolution of major small radicals (C_0 – C_2) in different bio-oil oxidation models during the ReaxFF MD isothermal simulations at 1900 K and 5 MPa (a) •CH_3 (b) HO_2•

Analysis shows that all the surrogate models have similar element composition that is very close to the 24-component bio-oil model. By comparing the simulation results, it is shown that model #3 can better reproduce the evolution of fuel and O2; Model #4 has better reproducibility for evolution profiles of CH2O, C2H2O and •CH3; CO evolution is best reproduced by model #2, while H2O by model #5.
This work demonstrates a methodology for investigating the high temperature oxidation pathways of complex fuel systems with ReaxFF MD simulations permitted by the comprehensive reaction analysis capability of VARxMD[1]. It is also a new attempt to have bio-oil surrogate models evaluated with ReaxFF MD simulation, which should be more feasible an approach for validation of surrogate chemical property theoretically[2].
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References:
[1] Jian Liu, Xiaoxia Li, Li Guo, Mo Zheng, Junyi Han, Xiaolong Yuan, Fengguan Nie, Xiaolong Liu. Reaction Analysis and Visualization of ReaxFF Molecular Dynamics Simulations. Journal of Molecular Graphics and Modelling 2014, 53(9)13-22
[2] Song Han, Xiaoxia Li, Mo Zheng, Li Guo, Initial reactivity differences between a 3-component surrogate model and a 24-component model for RP-1 fuel pyrolysis evaluated by ReaxFF MD. Fuel 2018, 222, 753-765