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REACTIVE MOLECULAR DYNAMICS OF ALTERNATIVE FUELS FOR LIQUID PROPULSION SYSTEMS

Abstract

The present work presents the simulation of the pyrolysis and combustion of alternative fuels, suitable for aerospace applications in liquid rocket engines, by Reactive Molecular Dynamics methods. There is a comparison among farnesane, alpha-farnesene and beta-farnesene, all of them obtained from the fermentation of sugars present in sugarcane juice. The pyrolysis mechanisms were elucidated for all compounds. There are significative differences among the reactions and processes observed during the decompositions. Using a first-order approach, the Arrhenius parameters of the global process were obtained with three different temperatures (held constant over time). For the pyrolysis, the obtained activation energies of farnesane, alpha-farnesene and beta-farnesene were 132.55, 117.28 and 112.88 kJ mol-1, respectively, and for the combustion, the obtained Ea were were 71.63, 37.99 and 37.98 kJ mol-1, respectively. Thermodynamic parameters were also estimated using Eyring equation, therefore enabling the calculation of the enthalpy, entropy and Gibbs energy. All data obtained are compatible with the ones found in the literature for hydrocarbon fuels, thus proving the usefulness of these compounds as green liquid fuels for rocket propulsion.