Combustion behavior and kinetics of tackifying resin by TG-FTIR and DFT analysis to assess the waste-to-energy potential

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Abstract

The combustion behavior and kinetics of tackifying resins (such as glycerol ester of colophony/hydrogenated colophony and C9/hydrogenated C9 petroleum resin, namely GEC, GEHC, C9PR and HC9PR, respectively) were investigated by TG-FTIR and density functional theory (DFT) analyses. The calorific values of different resins are higher than that of standard coal, indicating tackifying resins and their wastes are a promising fuel for generating energy. The average activation energies obtained by Friedman method for GEC, GEHC, C9PR and HC9PR were 223.51, 162.16, 166.52 and 116.20 kJ/mol, respectively, revealing that (H)C9PR were more readily combustible than GE(H)C, and their hydrogenated products burned more easily than their unhydrogenated ones, which were strongly supported by the TG-FTIR results. DFT calculations also show that the bond dissociation energy of C-C bond of GEC is higher than those of C9PR and GEHC. The best appropriate reaction mechanism evaluated by the master plots method is R3 model.

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Graphical Abstract