Automating the Pyrolysis Model Development Process

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Pyrolysis models are valuable tools for understanding material flammability and modeling fire growth. However, the development of comprehensive pyrolysis models is difficult and time-consuming due to the sheer number of material parameters required. Previous parameterization attempts employ massively parallel optimization problems using heuristic search algorithms to solve, but have been criticized of lacking physical significance and having reduced accuracy outside of calibrated ranges. This work sought to improve upon a previously developed method wherein the experimental results of both milligram- and bench-scale tests are inversely analyzed in a hierarchical approach. Three steps in the hierarchical process are automated using simple steepest ascent hill climbing optimization algorithms. The novelty of this approach lies in the custom fitness criteria and highly constrained and physical significant search space resulting from well-defined experiments. Two distinct materials were studied to evaluate the methodology: poly(methyl methacrylate) and rigid polyisocyanurate foam. The optimization programs were able to achieve 99% fits of both mass loss rate (MLR) from thermogravimetry (TGA) experiments and back surface temperature histories from Controlled Atmosphere Gasification Apparatus (CAPA II) experiments. Models were validated against independent MLR histories from CAPA II experiments under low and high heat fluxes.