Automated Characterization of Heat Capacities and Heats Of Pyrolysis Of Flammable Materials

Morgan C. Bruns, St. Mary's University / Isaac T. Leventon, NIST

A fully automated algorithm is presented for extracting temperature dependent specific heat capacities and heats of pyrolysis from differential scanning calorimetry (DSC) data. This algorithm is part of a larger project aimed at rapidly characterizing the material properties that are needed as inputs for fire models using experimental data from milligram and gram scale experiments in a hierarchical approach. Kinetic parameters from thermogravimetric analysis are assumed as this algorithm is one part of a multicomponent open source toolbox implemented in the Python programing language. This fully automated methodology is significantly more efficient than current analysis approaches. Verification is accomplished by applying the script to manufactured DSC data for one- and two-step reaction mechanisms. The script is validated by comparison to experimental data for a range of synthetic polymers. For each of these materials, a full set of specific heat capacities and heats of pyrolysis are presented.