AUTOMATED CHARACTERIZATION OF PYROLYSIS KINETICS AND HEATS OF COMBUSTION OF FLAMMABLE MATERIALS

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ABSTRACT

A fully automated algorithm is presented for extracting pyrolysis kinetic parameters and heats of combustion from a coupled analysis of thermogravimetric analysis (TGA) and microscale combustion calorimetry (MCC) data. This algorithm is part of a larger project aimed at rapidly characterizing the material properties that are needed as inputs for fire models. The algorithm is based upon an iterative analysis of the peaks in the derivatives of the TGA data and an approximate solution of the governing kinetic equations. The algorithm is implemented as a script in the Python programming language. The algorithm determines an effective decomposition mechanism (consisting of one, or multiple, decomposition steps), associated Arrhenius reaction rate kinetic parameters (A_i and E_i), and heats of combustion of the gaseous volatiles produced by individual reaction steps. This fully automated methodology is significantly more efficient than current analysis approaches—a full set of kinetic parameters is produced in less than one second. Verification is accomplished by applying the script to manufactured TGA and MCC data for one- and two-step reaction mechanisms. The script is applied to experimental data for cast poly(methyl methacrylate) (PMMA), acrylonitrile butadiene styrene (ABS), Kydex, Nylon 6,6, a flexible polyurethane foam (FPUF), polyvinyl chloride (PVC), and the leaves of lodgepole pine and Douglas fir trees. For each of these materials, a full set of kinetic parameters and heats of combustion are presented.