A Thermo-Kinetic Model of Pyrolysis

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A number of mathematical models have been developed to describe degradation of solid materials exposed to external heat. These models range in complexity from analytical formulations based on a steady-state approximation to complete numerical solutions of transient heat and mass transport coupled with chemical reactions. Potentially, these models can be used to understand and predict materials flammability. However, their utilization has been hampered by reliance on sets of assumptions that makes each of them applicable to a relatively narrow range of conditions and limited number of materials. This situation is further complicated by the fact that for most of these models the exact boundaries of applicability have not been established. The purpose of this work is to develop a computational tool that is capable of modeling pyrolysis and combustion of a wide range of materials under the conditions encountered in bench-scale flammability tests (cone calorimetry, flame spread, UL-94). The model is termed thermo-kinetic because it combines transient thermal energy transport and material transformations described by means of chemical kinetics. The model also includes a simplified description of transport of gases through the condensed phase. It is capable of capturing important aspects of material behavior such as charring and intumescence. The complexity of the model can be adjusted by introducing or removing material components with specified physical and chemical properties. Currently, a one-dimensional version of this model is being developed that will be expanded to include a two-dimensional simulator of flame spread. In both cases, a detailed description of condensed-phase processes will be coupled with a simple, empirical description of energy feedback from the flame.