Using Genetic Algorithms to Derive the Parameters of Solid-Phase Combustion from Experiments

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Introduction

The controlling mechanisms in the combustion of solid fuels is of great interest to fire safety. Numerical modeling is very useful for forensic reconstruction and prediction of fire characteristics (ignition resistance, propagation speed, heat release rate, production rate of toxic products). It also provides a cost-effective alternative to certain types of experimental test, particularly material flammability evaluation in reduced gravity environments (i.e. spacecrafts).

As numerical models of combustion increase in complexity, they require a larger number of fundamental material properties (or model parameters) to describe the underlying physical and chemical mechanisms. Some of these parameters are difficult to define with certainty for thermally degrading solids, especially for those with complex fire-behaviour such as polymers.

The proposed methodology involves simulating experimental tests with a theoretical model and using a genetic algorithm to find a set of model parameters (material properties) that provide the best agreement between the model predictions and the experimental data. The methodology is applied to two solid-combustion phenomena: smoldering propagation in polyurethane foam and flaming ignition/combustion of wood and of polypropylene.

Genetic Algorithms

Classical optimization tools are not appropriate for the present application because the high dimensionality of the problem produces a large search-space and very complicated landscapes of the optimization target, with numerous local maxima and minima. An efficient multidimensional optimization technique such as a genetic algorithm (GA) is therefore necessary.

GAs are a heuristic search method that imitates the principles of biological adaptation. Its simple and robust mechanism of optimization is based upon the mechanics of the Darwinian survival-of-the-fittest theory [Goldberg]. Contrary to classical optimization methods for non-linear problems (trial and error, least squares, gradient method, random strategies, and solution mapping), GAs can efficiently handle high multidimensionality, intricate or non continuous objective-landscape, multiple local optima, and noise in the data. GAs are found to be valuable for several engineering problems and have been applied to derive chemical kinetics, with a bigger emphasis on homogeneous gas-reactions [Polifke].

Smoldering Kinetics of Polyurethane Foam

Smoldering is a flameless, surface combustion reaction, deriving its heat from heterogeneous oxidation of the solid fuel. Smolder-initiated fires are the leading cause of fire deaths in the United States [Hall].

PU foam is a common material used in upholstered furnishings and a major fire-safety concern due to its low ignition-resistance to smolder. The majority of the studies on PU thermal-decomposition lack complete information valid for numerical models of smoldering. Furthermore, accept mechanisms of PU smoldering do not universally describe smoldering for all propagation modes, and different mechanisms are required depending if it is forward or opposed smolder. This work establishes a PU kinetic mechanism that is valid for both propagation modes.

Previous thermogravimetric (TG) experiments [Chao] are used to explore the thermal degradation of PU and develop a new reduced mechanism consisting on: two pyrolysis of the foam; two oxidations of the foam to form char; and oxidation of the char. Assuming Arrhenius reaction-rates, sixteen kinetic parameters are required: four activation energies, four preexponential factors, four reaction-order coefficients, and four stoichiometric yields. Using a Genetic Algorithm, numerical simulations of solid mass-loss are systematically compared to experiments, thus allowing the determination of the kinetic and stoichiometric parameters that provide the best agreement. It is found that the proposed mechanism and the calculated parameters work well for TG simulations at different heating rates (5, 10, and 20 °C/min) and oxygen concentrations (nitrogen and air atmospheres).

To verify that the reduced mechanism proposed above is comprehensive to capture the smolder behavior, a propagating smolder-front is modeled. The model is one-dimensional and steady state, and only the species conservation equations are solved. The results show that using a single kinetic mechanism, the model predictions are in phenomenological agreement with experimental results in both opposed and forward smolder.

Flaming Ignition and Combustion of Solids

One of the biggest impediments to fire growth modeling is our limited ability to use data from common bench-scale fire tests, such as the Cone Calorimeter [ASTM E1354] to characterize practical materials in terms of the solid phase "material properties" needed by simplified numerical pyrolysis models.

The NIST FDS v4.0 [McGrattan] pyrolysis model is used to calculate the material surface temperature and mass loss rate histories as a function of the material properties. A GA based on the processes of natural selection and mutation is developed and integrated with the pyrolysis model. The combined GA/pyrolysis model is used with Cone Calorimeter data [Hopkins] to estimate the material properties for two charring materials (redwood and red oak) and one thermoplastic material (polypropylene).

The results show that there is good agreement between the model predictions and the experimental data prior to ignition. This is encouraging because with this approach, all properties needed to characterize a material for fire modeling can be estimated from a single bench-scale fire test.

Conclusions

The feasibility of using a Genetic Algorithm to estimate material properties from common test data has been demonstrated. The parameters (material properties) were automatically adjusted to find a parameter set that provides near-optimal agreement between the model predictions and the experimental data given the constraints imposed by the physical models.

Parameters of thermal degradation and fire behavior are needed for numerical modelling of solid combustion but not easily available. The methodology proposed here can be further applied to other materials, or to estimate other material properties, i.e. enthalpies of reaction from calorimetry or heat release experiments.

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