Computer Models For Fire and Smoke

Model Name: ThermaKin2D

Version: 3

Date: February 26, 2014

Model Actively Supported? Actively updated, yes; active user support/FAQs, no.

Classification: Condensed Phase Material Degradation and Pyrolysis; Flame Spread

Very Short Description: A quantitative understanding of the processes that take place inside a burning material is critical for predicting the ignition and growth of fires. To improve this understanding and enable predictive modeling, a numerical pyrolysis solver called ThermaKin was developed. This solver computes the transient rate of gaseous fuel production from fundamental physical and chemical properties of constituents of a pyrolyzing solid. It was successfully applied to the combustion simulation of a broad range of materials. One limitation of ThermaKin was that it could handle only one-dimensional burning problems. As a consequence, flame spread, which is an important contributor to fire growth, could not be simulated. This technical note presents a new computational tool, ThermaKin2D, that expands the ThermaKin model to two dimensions and combines it with a flexible analytical representation of a surface flame. It is expected that this tool will enable highly accurate simulations of flame-spread dynamics. This technical note contains a description of this new computation tool, reports results of a series of verification exercises, and demonstrates some of the ThermaKin2D capabilities.

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User's Guide: DOT/FAA/TC-TN12/59
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This document is also available from the Federal Aviation Administration William J. Hughes

Technical Center at actlibrary.tc.faa.gov.

Technical References: see above

Validation References: Stoliarov, S. I., Leventon, I. T., and Lyon, R. E., **Two-dimensional model of burning for pyrolyzable solids**, *Fire and Materials*, 2013.

Availability: By Request, stolia@umd.edu

Price: Free

Necessary Hardware: A single instance of the program is designed to run on a single processor (or core) and may require up to several gigabytes of random-access memory (the memory requirement depends on the number of components and number of elements in the object).

Computer Language: ThermaKin2D is implemented using ANSI/ISO C++ and its standard library.

Size: 208 kB

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Detailed Description:
It has been recognized that the processes that take place in the condensed phase of a burning material play a pivotal role in the overall combustion [1]. A quantitative understanding of these processes is critical for prediction of ignition and growth of fires. During the past several years, a number of detailed numerical models that predict the rate of gaseous fuel production (or burning rate) from fundamental physical and chemical properties of constituents of a pyrolyzing solid have been developed. Examples of such models include Gpyro [2], solid phase solver within the Fire Dynamics Simulator [3]; and ThermaKin [4], which was developed by the Federal Aviation Administration. These models have similar capabilities—they solve transient conductive and radiative energy transfer coupled with decomposition chemistry. Gpyro and ThermaKin also include the transport of gaseous decomposition products inside the condensed phase and associated convective heat flow. The main distinctive feature of ThermaKin is a flexible kinetics solver that can handle chemical mechanisms consisting of up to 30 first- and second-order reactions (including those between two different reactants). Most of the newly designed flame-resistant materials are multicomponent polymeric systems with complex thermal degradation chemistry [5]. Thus, from the prospective of a fire-resistant material developer, ThermaKin represents the most suitable modeling tool.

ThermaKin has been successfully applied to the combustion simulation of noncharring [6] and charring polymers [7] in a cone calorimetry-type scenario [8]. In both cases, the model was parameterized using mg- and g-scale property measurement techniques. A simple, empirical formulation was employed to capture heat feedback from the surface flame. The burning rate and temperature histories of material samples exposed to a uniform radiant heat flux were predicted.

The cone calorimetry scenario was essentially one-dimensional, which made it a convenient simulation target. However, this scenario does not include the process of surface flame spread, which has been identified as a critical determinant of the rate of fire growth [9]. Flame-spread phenomenon was studied extensively by a large number of researchers, including de Ris [10]; Fernandez-Pello and Hirano [11]; Quintiere, et al. [12]; and Ito and Kashiwagi [13]. Nevertheless, the ability to predict this phenomenon from fundamental physical and chemical properties of a burning solid remains limited.

The FAA technical note discusses this new computational tool, ThermaKin2D, which extends ThermaKin modeling framework to the simulation of flame spread. ThermaKin2D expands the condensed-phase pyrolysis model to two dimensions and combines it with a flexible analytical representation of a surface flame. The flame model is based on highly, spatially resolved measurements of the heat feedback from a flame spreading vertically on poly(methyl methacrylate) [13 and 14]. It is expected that coupling this flame model with a detailed pyrolysis solver will enable highly accurate simulations of the spread dynamics. This technical note contains a mathematic description of the new model, reports results of a series of verification exercises, and demonstrates some of the Thermakin2D model’s capabilities.

REFERENCES

1. Kashiwagi, T., "Polymer Combustion and Flammability—Role of the Condensed Phase," *Twenty-Fifth Symposium (International) on Combustion,* 1994, pp. 1423-1437.
2. Lautenberger, C. and Fernandez-Pello, C., "Generalized Pyrolysis Model for Combustible Solids," *Fire Safety Journal,* Vol. 44, 2009, pp. 819-839.
3. McGrattan, K., Hostikka, S., Floyd, J., Baum, H., Rehm, R., Mell, W., and McDermott, R., "Fire Dynamics Simulator (Version 5) Technical Reference Guide," National Institute of Standards and Technology Special Publication, 2007.
4. Stoliarov, S.I. and Lyon, R.E., "Thermo-Kinetic Model of Burning," Federal Aviation Administration Technical Note, DOT/FAA/AR-TN08/17, 2008.
5. 2012 American Chemical Society Spring National Meeting, *Fire and Polymers Symposium*, San Diego, California, March 2012.
6. Stoliarov, S.I., Crowley, S., Lyon, R.E., Linteris, G.T., "Prediction of the Burning Rates of Non-Charring Polymers," *Combustion and Flame,* Vol. 156, 2009, pp. 1068-1083.
7. Stoliarov, S.I., Crowley, S., Walters, R.N., Lyon, R.E., "Prediction of the Burning Rates of Charring Polymers," *Combustion and Flame,* Vol. 157, 2010, pp. 2024-2034.
8. ASTM E 1354 – 09, "Standard Test Method for Heat and Visible Smoke Release Rates for Materials and Products Using an Oxygen Consumption Calorimeter," ASTM International, West Conshohocken, Pennsylvania, 2009.
9. Quintiere, J.G., *Fundamentals of Fire Phenomena,* John Wiley & Sons, Chichester, United Kingdom, 2006.
10. De Ris, J.N., "Spread of Laminar Diffusion Flame," *Twelfth Symposium (International) on Combustion*, 1969, pp. 241-252.
11. Fernandez-Pello, A.C., Hirano, T., "Controlling Mechanisms of Flame Spread," *Combustion Science and Technology,* Vol. 32, 1983, pp. 1-31.
12. Quintiere, J., Harkleroad, M., Hasemi, Y., "Wall Flames and Implications for Upward Flame Spread," *Combustion Science and Technology,* Vol. 48, 1986, pp. 191-222.
13. Ito, A., Kashiwagi, T., "Characterization of Flame Spread over PMMA Using Holographic Interferometry Sample Orientation Effects," *Combustion and Flame,* Vol. 71, 1988, pp. 189-204.
14. Leventon, I.T., Stoliarov, S.I., "Evolution of Flame to Surface Heat Flux During Upward Flame Spread on Poly(methyl methacrylate)," *Proceedings of the Combustion Institute,* in press.