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INTERFACING MATERIALS MODELS WITH FIRE FIELD MODELS

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ABSTRACT

For flame spread over solid materials, there has traditionally been a large technology gap between fundamental combustion research and the somewhat simplistic approaches used for practical, real-world applications. Recent advances in computational hardware and computational fluid dynamics (CFD)-based software have led to the development of fire field models. These models, when used in conjunction with material burning models, have the potential to bridge the gap between research and application by implementing physics-based engineering models in a transient, multi-dimensional tool. This paper discusses the coupling that is necessary between fire field models and burning material models for the simulation of solid material fires. Fire field models are capable of providing detailed information about the local fire environment. This information serves as an input to the solid material combustion submodel, which subsequently calculates the impact of the fire environment on the material. The response of the solid material (in terms of thermal response, decomposition, charring, and off-gassing) is then fed back into the field model as a source of mass, momentum and energy. The critical parameters which must be passed between the field model and the material burning model have been identified. Many computational issues must be addressed when developing such an interface. Some examples include the ability to track multiple fuels and species, local ignition criteria, and the need to use local grid refinement over the burning material of interest.

KEY WORDS: Solid Material Combustion, Fire, Modeling

1. INTRODUCTION

Solid material decomposition models and flame spread models have been the focus of much research. There have been many excellent works on flame spread (e.g., [1]-[6]). The first two references contain good reviews of the subject, which will not be repeated here. Traditionally, models that require many simplifying assumptions have been developed to predict how a solid combustible will decompose under a given heat flux and subsequently burn. Because of the complexity of the decomposition and flame spread processes, these methods have been limited in their ability to include all of the important physics. For example, some of the early models of flame spread in room fires neglected the radiative feedback from the flame and hot gas layer to the combustible surface. Others were limited to very simplistic geometries (e.g., a vertical wall with no ceiling above it). Also, many of these models have been derived based on bench-scale

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data, and do not, in general, scale to real-world applications. This can be understood by noting the importance of edge effects in Cone Calorimetry data. Also, while there is a large amount of large-scale experimental data, the fact that it is material- and scenario-specific makes it difficult to directly apply it to model development.

To capture the complexity of the solid material decomposition and flame spread processes, numerical models of upward flame spread have been developed (e.g., [7]-[8]). Similarly, numerical models of the lateral flame spread problem have been developed (e.g., [9]-[10]). Some of these efforts were primarily concerned with very small-scale studies, and are not directly applicable to the modeling of a room fire. These models have increased the level of fidelity to the solid material decomposition physics, but fall short in coupling the solid material behavior to the overall environment (such as to the hot gas layer and local burning effects in a room fire). The fire environment must be known (specified as inputs or boundary conditions) for such models.

Fire *field* models are CFD-based models that solve the governing equations of energy, mass, and momentum transport from a 'first principles' basis. Since their roots are in computational *fluid* dynamics, fire field models have been primarily applied to model the transport of smoke and hot gases generated by the fire ([11]-[13]). Over the past 10 years, engineering combustion models (for gaseous or liquid fuels) have been developed and incorporated into fire field models, along with engineering models for soot generation and combustion, and thermal radiation. The result is that fire field models are being applied to more than just smoke and heat transport, and now are capable of modeling the fire itself (not just the products of fire). These models have provided useful insights into the complex phenomena that comprise a fire ([14]-[16]).

Since fire field models have demonstrated their utility for understanding complex physical mechanisms in large gaseous and liquid fuel fires, efforts are underway to broaden the range of applicability of fire field models to include fires resulting from the decomposition of solid materials. Opstad [17] has modified a fire field model to include a solid material combustion model that uses Cone Calorimetry data as input. This pioneering work has been used to investigate the upward flame spread problem for a tunnel fire. The drawbacks of Opstad's method are that it is limited to Cone Calorimeter data, and also that is uses propane to represent the solid material pyrolysis products. The drawbacks to Cone Calorimeter data are that it strictly applies only to low heat fluxes, small sample sizes, and a specific orientation and boundary conditions. A similar effort (which also utilizes Cone Calorimeter data) has been underway in Sweden [18]. Room fires have been investigated, and the need to develop and implement a better representation of the pyrolysis process into the fire field model has been noted. Additionally, work by Moss and colleagues [19] is underway to investigate polymer fires with a fire field model.

The need to interface solid material combustion models with fire field models has been demonstrated in the international fire community. Recent efforts by the present authors have focussed on developing such an interface for a particular fire field model.The purpose of this paper is to elucidate the coupling that is necessary between fire field models and solid material combustion models for the modeling of room-scale solid material fires. Its goal is to point out some of the technical difficulties that must be dealt with in the development of such models, and to identify the types of experimental data needed to support this development.

2. METHODOLOGY

The methodology required to couple a solid material combustion model with a fire field model will be somewhat a function of the particular models that are to be coupled. The methodology described herein is based on the authors' experience with the VULCAN[2] fire field model, but is believed to be applicable to the majority of fire field models that are presently in existence. While the present work assumes that existing models are to be interfaced, the same considerations would be necessary for someone undertaking the development of a new, integrated model from scratch.

In general, due to the complexity of the fire field model, one will want to interface the solid combustible model and the field model in such a way as to minimize the impact on the fire field model. The flow chart shown in Figure 1 depicts the areas of the field model that must be modified to incorporate the solid material combustion model. The flow is meant to represent the flow of information and processes in a typical field model, and not the flow of effort in the development of the coupled models. First, the user must have a convenient way of entering the important solid material combustion parameters into the model. This is generally done via a pre-processor, which virtually all field models rely upon for geometry and data input. Assuming that a pre-processor already exists as an integral part of the field model, modifications must be performed to allow the user to also include solid material combustion information. The particular set of parameters which must be input will be a function of the solid combustion model that is to be interfaced with the field model. For example, the following parameters are input via a pre-processor to interface a simple char model with VULCAN: a means of designating which cells in the finite difference grid are solid combustibles, the thickness of the solid combustible material, and the thermo-physical properties of interest (heat of chemical decomposition, pyrolysis temperature, ignition temperature, virgin and char densities, conductivities, specific heats, absorption coefficients). The decomposition products from the pyrolysis process, and the associated heat of combustion of those products, must either be specified via the pre-processor, or calculated as part of the solid material combustion model.

Once the needed input information has been obtained, initialization of the new variables that have been introduced must occur. Then the computations can begin. Many field models (e.g., VULCAN) will calculate the thermal response of objects and their impact on the local flow field and radiation fields. Solid combustible materials may require a different treatment, since they can produce energy, mass, and momentum sources in the flow. Also, a different (perhaps more detailed) conduction algorithm may be required for solid combustibles in order to accurately model the pyrolysis and ignition processes. Assuming this to be the case, there must be some 'check point' in the model to determine whether a solid object is combustible or not.

For solid combustible objects, submodels must be added to the field model for all of the phenomena of interest. These submodels will determine the mass, momentum, and energy sources that result from the solid combustible material. For example, as a minimum, one must add a thermal response submodel (unless an existing one is to be used), a pyrolysis submodel (to determine the mass loss rate, and perhaps the properties of the decomposition products), and a submodel for the change in thermo-physical properties of the virgin/char material versus temperature. If one is interested in accounting for the change in solid combustible thickness with time, then this must be included in the above submodels. The solid combustible thermal response submodel that is most suitable for the general problem will likely be of the finite difference (or finite element) type. These models alone possess the generality to handle the complexities of the fire problem: temperature dependent properties, char/virgin materials, chemical effects within the solid combustible, radiation and convection boundary conditions, endothermic/exothermic reactions within the material, and changing material thickness.

Once the mass, energy, and momentum sources that result from the combustible material have

2. VULCAN is under joint development at Sandia National Laboratories and SINTEF/NTH (Norway), and is based on KAMELEON II Fire developed at SINTEF/NTH.

been determined, they must be added into the mathematical equations that the field model solves. This is done by modifying the coefficients and source terms of the equations for mass, energy, and momentum conservation to reflect the contributions from the solid combustible material. Note that these source terms appear in the fluid cells that are adjacent to the solid combustible, and not in the solid material itself.

If the field model is not general enough to handle an arbitrary number of fuel and inert species, it will also be necessary (in general) to modify the number of fuels and species which the field model can handle. Scenarios of interest (e.g., a room fire) generally involve an initiating (primary) fuel (such as a waste basket fire, or small pool fire) which ignites wall materials (secondary fuel). Unless the wall material pyrolysis products can be assumed to be the same as the pool fire volatiles (not a good assumption for the general case), then the field model must be able to handle at least two types of fuels. Similarly, inert products of the pyrolysis process can differ substantially from nitrogen, and must be accounted for by the field model.

One final modification is required. The fire field model must have some way of recognizing that ignition can occur near a solid combustible surface, and also igniting the adjacent fuel/air volume if appropriate. In many field models, ignition is generally at a user-specified location (or locations). The ability to propagate the combustion process once ignition has occurred is generally not a problem with most fire field models. But most models have not been developed to ignite gas volumes adjacent to hot surfaces. Therefore, some modification is needed to include ignition near surfaces. Of course, there are several possible ignition criteria that can be specified (see for example [20]), and a choice must be made as to which one is most appropriate for the problems of interest.

3. DISCUSSION

The methodology described above appears to be straightforward, and generally applicable to most fire field models and solid combustible models, although deviations could be necessary depending on the particular models that are being interfaced. However, there are many underlying issues which complicate the interfacing of a fire field model and a solid material combustion model. Some of these issues will be discussed in this section, to highlight the detailed consideration necessary to interface these types of models.

The methodology described above has been focussed primarily on upward flame spread processes. The modeling of lateral flame spread (also called creeping flame spread) requires special considerations since the physics which drive the lateral flame spread process are very different than for the upward case. The lateral flame spread is driven by thermal conduction at the interface between the fuel, air, and solid, and therefore has controlling physical processes occurring on length scales that are small relative to the upward flame spread mechanisms. While it is relatively easy to capture the upward flame spread mechanisms on a finite difference grid developed for the fluid flow problem, a substantially finer grid would be required to accurately track the lateral flame spread process across the solid surface. If the entire domain of the problem of interest consists only of a small section of burning combustible, such a fine grid does not represent any difficulty. Numerical solutions to such problems have been demonstrated in the literature (e.g., [9]-[10]). However, if the problem of interest is a room fire, it could be computationally prohibitive to use the fine grid resolution required to resolve the lateral mechanisms. If one is primarily interested in the upward flame spread, but also wants (secondarily) to include the lateral flame spread, it may be possible to include the lateral flame spread via empirical relationships or submodels present in the literature (e.g., [21]-[23]). Such models would be 'subgrid' models, i.e., the small scales involved are not resolved on the grid, and must therefore be accounted for using an engineering model within each grid cell.

A second issue that must be resolved in implementing the above methodology is a conceptual one: since the field model already handles solid obstacles, should the solid combustible be included as another type of solid obstacle, or simply as a lining material present on the face of an existing obstacle? This decision will be influenced by both the particular field model involved, and also the solid combustible model attributes desired. If one is interested in modeling the burning of logs in a fireplace, it is easiest to conceptualize the problem as one in which the entire cell is a solid combustible obstacle. On the other hand, if one is interested in modeling the burning of wall coverings, it is easier to conceptualize the problem as one in which the solid combustible is a lining on an existing obstacle cell (representing the wall). This conceptual choice will impact many of the details in the actual implementation of the solid combustible model/field model interface. For example, if the solid combustible represents a lining material on an obstacle, then the solid combustible can be specified as existing on a limited number of faces of the cell. If the entire cell is a solid combustible, then all 6 faces of the cell (assuming the cell is a rectangular parallel-piped corresponding to a 3-dimensional cartesian grid) would be combustible. Also, if a solid combustible material is conceptualized as a lining material, then consideration must be given as to how the solid combustible thickness will enter the fluid flow and thermal transport problems. Changes in the solid combustible thickness with time are not difficult to include for the thermal conduction problem, but can be very difficult to include for the fluid flow and radiation aspects of the problem. An adaptive grid would be required to include such physics.

A third issue involves the additional fuels and species that the solid combustibles add to the fire problem. As discussed in the Methodology section, the fire field model must be able to handle these additional fuels and species. This procedure is not always straightforward, depending on the fire field model employed. The coupling of the enthalpy and species source terms must be very tight in a fire field model: i.e., there can be very little imbalance between the two, or mass and energy will no longer be conserved. The problem of accurate conservation increases substantially as the number of fuels and species increases. This may necessitate that a completely new algorithm be formulated for the energy and species conservation, or that a new solution scheme be adopted. Beyond this possible difficulty, there is another significant hurdle. The pyrolysis products and their rate of evolution are not known for most real-world materials. This level of detail has generally not been obtained in the modeling of pyrolysis, perhaps because very few models have required such detail to date. For some solid combustible materials, the pyrolysis products can be a strong function of time, as well as of heat flux and local flow field. One can envision that the relatively light volatiles will be released early in the pyrolysis process, while the heavier volatiles are released later in the process from the charred material. It is also known that trace quantities of some additives can have a dramatic effect on the composition and rate of production of pyrolyzates [20]. Data and models on the time-dependent composition of off-gases and the thermophysical properties of the constituent gases are required to support the coupling of fire field models with burning material models.

One final issue for consideration is the finite difference (or finite element) grid that will be used in the combined fire field model/solid combustible model. Some comments in this regard have been made previously herein regarding upward versus lateral flame spread. Grid resolution can also be important for the upward flame spread process. A grid which is too coarse will be unable to accurately resolve ignition and solid combustible burning area. Grid issues are also important regarding the solution of the conduction problem within a solid combustible cell (i.e., in-depth). As pointed out earlier, a finite difference technique (or finite element) may be best suited for the solution of the conduction problem within a solid combustible cell. The selection of an appropriate grid for the in-depth conduction problem depends on the problem of interest. For accurate resolution of the ignition and flame spread problem, a grid which is relatively fine near the material surface is required. However, for accurate calculation of the pyrolysis rate, a grid which is refined near the pyrolysis front and moves with the pyrolysis front would be better. The optimal grid (in-depth as well as over the solid combustible surface) will be problem dependent.

4. CONCLUSIONS

The methodology required to couple solid material combustion models to a fire field model has been outlined, and appears to be relatively straightforward. However, there are a number of issues that must be addressed in the actual implementation of the methodology. None of the issues raised make the coupling of fire field models and solid combustion models intractable, but they do indicate that many implementation issues must be addressed in the development of such models. The success or failure of using fire field models for problems involving solid material combustibles will depend on the manner in which these issues are addressed. Additionally, the experimental data and model development which are needed to interface solid material combustion models with fire field models have been identified.

5. REFERENCES

1. F.A. Williams, Sixteenth Symp. (Int.) on Comb., Pittsburgh, (1976).

2. A.C. Fernandez-Pello and T. Hirano, Comb. Sci. & Tech., 32, 1, (1983).

3. A.C. Fernandez-Pello, Comb. and Flame, 31, 135, (1978).

4. J.G. Quintiere and M. Harkleroad, Fire Safety Science and Engineering, ASTM, Philadelphia (1985).

5. K. Saito, J.G. Quintiere, and F.A. Williams, First Int. Symp. on Fire Safety Sci, pp.75, (1986).

6. J.N. de Ris, Twelfth Symp. (Int.) on Comb., pp.241-252, (1969).

7. M.A. Delichatsios and Y. Chen, Fourth Int. Symp. on Fire Safety Sci., pp.457-468, (1994).

8. M.M. Delichatsios, M.K. Mathews, and M.A. Delichatsios, Third Int. Symp. on Fire Safety Sci., (1991).

9. C. DiBlasi, S. Crescitelli, and G. Russo, Combust. Flame, 72, 205, (1988).

10. S. Bhattacharjee and R.A. Altenkirch, Twenty-Fourth Symp. (Int.) on Comb., pp. 1669-1676, (1992).

11. G. Cox and S. Kumar, Comb. Sci. & Tech., 52, pp. 7-23, (1987).

12. S. Nam and R.G. Bill, Jr., Fire Safety J., 21, pp. 231-256, (1993).

13. K.T. Yang, H.J. Huang, and V.F. Nicolette, Heat Transfer in Fire and Combustion Systems, ASME HTD vol. 272, pp.13-20, (1994).

14. J. Holen, M. Brostrom, and B.F. Magnussen, Twenty-Third Symp. (Int.) on Comb., pp. 1677-1683, (1990).

15. L.A. Gritzo, V.F. Nicolette, D. Murray, J.L. Moya, and R.D. Skocypec, The Symp. on Thermal Sci. and Eng. in Honor of Chancellor C.L. Tien, November 14, (1995).

16. L.A. Gritzo, V.F. Nicolette, S.R. Tieszen, J.L. Moya, and J.Holen, Transport Phenomena in Combustion, Taylor & Francis (1995).

17. K. Opstad, Modeling of Thermal Flame Spread on Solid Surfaces in Large-Scale Fires, Dr. Ingeneur Thesis, Norwegian Inst. of Tech., Trondheim Norway, (1995).

18. Z. Yan and G. Holmstedt, CFD Simulation of Flame Spread in Room Fire, Presented at the First Euro. Symp. on Fire Safety Sci., Zurich, August 21-23, (1995).

19. J.B. Moss and C.D. Stewart, Flamelet Properties for the Field Modeling of Polymer Fires, Presented at the First Euro. Symp. on Fire Safety Sci., Zurich, August 21-23, (1995).

20. A.M. Kanury in SFPE Handbook of Fire Protection Engineering, NFPA, Quincy, MA, pp. 326-340, (1988).

21. Y. Chen and M.A. Delichatsios, Comb. and Flame, vol. 99, 601-609, (1994).

22. J.G. Quintiere, Fire Mater., 5:52, (1981).

23. A.C. Fernandez-Pello, S.R. Ray, and I. Glassman, Eighteenth Symp. (Int.) on Comb., p.579, (1981).

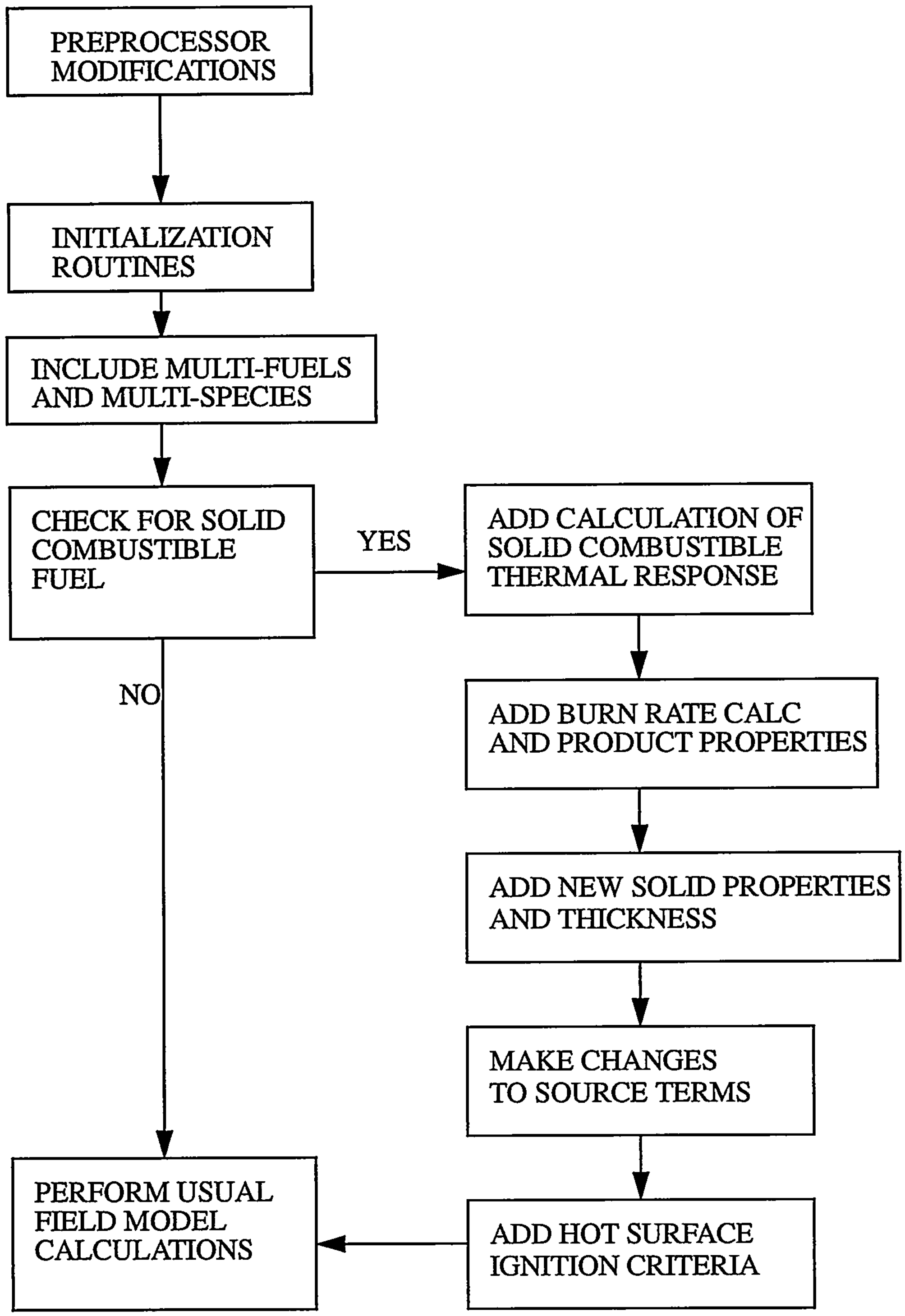

FIGURE 1: MODIFICATIONS NECESSARY TO FIELD MODEL METHODOLOGY TO INTERFACE IT WITH SOLID MATERIAL COMBUSTION MODEL