The Prediction of Fire Propagation in Enclosure Fires

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ABSTRACT

In this paper we present some early work concerned with the development of a simple solid fuel combustion model incorporated within a Computational Fluid Dynamics (CFD) framework. The model is intended for use in engineering applications of fire field modelling and represents an extension of this technique to situations involving the combustion of solid cellulosic fuels. A simple solid fuel combustion model consisting of a thermal pyrolysis model, a six flux radiation model and an eddy-dissipation model for gaseous combustion have been developed and implemented within the CFD code CFDS-FLOW3D. The model is briefly described and demonstrated through two applications involving fire spread in a compartment with a plywood lined ceiling. The two scenarios considered involve a fire in an open and closed compartment. The model is shown to be able to qualitatively predict behaviours similar to flashover - in the case of the open room - and backdraft - in the case of the initially closed room.

KEYWORDS: CFD, field model, pyrolysis, solid fuel combustion, flashover, backdraft

INTRODUCTION

Over the past 10 years considerable effort has been expended in developing fire field models capable of predicting the development of hazardous conditions within fire enclosures[1-4]. At the heart of these fire field models is the Computational Fluid Dynamics (CFD) code and a large proportion of these models are based on commercial CFD software such as PHOENICS[5] and FLOW3D[6]. The former is the core of the JASMINE[7] code and an aircraft cabin fire code[3] while the latter has been used to investigate the Kings Cross Underground fire[2] as well as aircraft[8] and high rise building fire scenarios[9]. The majority of practical fire modelling applications have been concerned with the spread of heat and smoke in complex structures and so

combustion has either been ignored or simplified. In cases where combustion is ignored the fire is treated as a simple prescribed source of heat and smoke. While this approximation may appear crude it can produce good agreement with experimentally derived temperature measurements[10,11] for room fire scenarios. Generally, when combustion is included, it is approximated using relatively simple one-step reaction mechanisms[12] for gaseous or liquid fuels such as methane.

While these combustion models increase the complexity of the simulation, they still ignore or greatly simplify many important combustion aspects. One of the major simplifications is the use of fluid rather than solid fuels. In these cases, in addition to the simplifications associated with turbulence, chemical mechanisms, reaction rate, soot formation and thermal radiation, the charring and pyrolysis processes, as well as the flame spread over solid surfaces are ignored.

While some recent work has attempted to predict fire spread in enclosures through the use of zone and field models [13,14], these have incorporated the rate of flame spread over the solid fuel through the use of thermal analysis and empirical formulations. Here we present a different approach, where the flame spread is governed by a set of partial differential equations which expresses gas phase behaviour, solid phase behaviour and their interaction. This paper represents early work concerned with the development of a simple solid fuel combustion model incorporated within a CFD framework. The model is being developed as a possible means of including simple solid fuel combustion considerations into practical engineering fire field models. Thus, relatively simple radiation and combustion models are considered here as a first approximation.

THE MATHEMATICAL MODELS

The models presented here have been incorporated within the CFDS-FLOW3D [6] software (Version 2.3.3). This is a general purpose CFD package which solves the set of three-dimensional, partial differential equations that govern fluid flow. This set consists in general, of the following equations: the continuity equation, the three momentum equations that govern the conservation of momentum per unit mass in each of the three space dimensions; the equation for conservation of energy; and, the equations for a turbulence model, in this case the k-epsilon model with buoyancy modifications. Compressibility is assumed and the perfect gas law is used to describe the equation of state. In this software, all solid surfaces are modelled with no-slip conditions for the velocities. The usual 'wall functions' are used to compute shear stresses at solid surfaces.

The combustion model consists of the following subcomponents, a gas phase combustion model, a radiation model and a thermal pyrolysis model. These will each be described in turn.

The Gas Phase Model

The governing equations for all fluid variables can be expressed in the general form:

$$\frac{\partial \rho \phi}{\partial t} + \operatorname{div}(\rho \vec{U} \phi) = \operatorname{div}(\Gamma_{\phi} \nabla \phi) + S_{\phi} \tag{1}$$

where S_{ϕ} is the source term and ϕ stands for any one of the following variables: the velocities u, v, w in three co-ordinate directions, the enthalpy h, the turbulent kinetic energy k, its dissipation rate ε , the mixture fraction ξ , and the mass fraction of fuel m_f . For continuity equation ϕ takes 1.

Combustion in the gaseous phase is modelled using the eddy dissipation concept[15]. A simple one-step chemical reaction, i.e., $F + v_o O \rightarrow (1 + v_o) P$ is assumed. The Lewis number is assumed to be 1. The source term of the governing equation for mass fraction of fuel employs the eddy dissipation concept, i.e.,

$$R_f = A \cdot \min(\bar{C}_f, \bar{C}_o / S) \frac{\varepsilon}{k}$$
 (2)

where A takes 4.0, S is the stoichiometric ratio of oxidant to fuel and $\bar{C_o}$ and $\bar{C_o}$ are the concentrations of fuel and oxidant respectively.

The Thermal Radiation Model

Flame spread over the surface of combustible materials is controlled by two central mechanisms—heat transfer to unburned material and gaseous chemical reaction[16]. Thermal radiation is the dominant mode of heat transfer in compartment fires. Thermal radiation from the fire and hot upper gas layer can heat the surrounding combustible materials to their pyrolysis temperature and provide the energy required for the pyrolysis process. As a first approximation, the six flux model[17] is used to describe thermal radiation.

The six radiation fluxes in the positive and negative directions x, y, z are denoted by F_x^+ , F_x^- , F_y^+ , F_y^- , F_z^+ and F_z^- respectively. Let $R_x = F_x^+ + F_x^-$, $R_y = F_y^+ + F_y^-$, $R_z = F_z^+ + F_z^-$. Then R_α is governed by the following second-order ordinary differential equation

$$\frac{d}{d\alpha} \left[\frac{1}{a+s} \frac{d(R_{\alpha})}{d\alpha} \right] = S_{\alpha}, \quad \alpha = x, y, z$$
 (3)

where $S_{\alpha} = R_{\alpha}(a+s) - 2a\sigma T^4 - s(R_x + R_y + R_z)/3$, α and s are the absorption and scattering coefficients respectively and σ is Stefan-Boltzmann constant.

According to Hubbard and Tien[18], the absorption coefficient a is a function of temperature T(K). Hubbard and Tien's curves for this dependence can be approximated using linear regression analysis. Using this approach the relationship between a and T can be roughly approximated by,

$$a = a_0 + b_0 T. (4)$$

For wood, a_0 and b_0 take 0.0517 and 0.00052 respectively. Using this relationship the absorption coefficient used in the radiation model becomes temperature dependent.

The Thermal Pyrolysis Model

Many efforts have been made to understand the chemical and physical process of pyrolysis[19]. The pyrolysis of solid fuels involves the complex process of chemical decomposition at very high temperature. During pyrolysis, the solid fuel may undergo melting, shrinking/expanding and charring. The thermal properties of the material will also vary with temperature. Several models have been developed to represent this complicated process[20,21,22]. The most complex of these models makes use of kinetic rate laws[21,22] and a large number of material properties[21]. Compared with these more sophisticated models, the thermal pyrolysis model[20] uses the relatively simple concept of the pyrolysis temperature as a first approximation. The relative simplicity of this model makes it an attractive proposition for engineering applications. This simple pyrolysis model is adopted in this paper. The pyrolysis mechanism is simply described as a process in which combustible gases are given off the surface of the solid fuel at the pyrolysis temperature. While the concept of the pyrolysis temperature is questionable and scenario specific, both physical experiments[23] and theoretical analysis[24] have demonstrated that it provides a fair approximation to the pyrolysis process for various materials.

In this model, combustible gases are released from the surface of the solid fuel when it is heated to its pyrolysis temperature T_p . In fires, the energy to sustain this endothermic gasification process is generally supplied by the thermal radiation emitted from the fire and hot combustion products. The rate of burning is expressed as

$$\dot{m}^{"} = \dot{q}^{"}/L \tag{5}$$

where \dot{q} is the net heat flux reaching the solid surface and L is the heat of pyrolysis. The model also includes the following assumptions:

- 1) thermal properties of the solid fuel are independent of temperature;
- 2) the material does not melt, shrink/expand or char;
- 3) combustible gases are blown-off the solid surface with a zero initial velocity;
- 4) solid mass losses of the target fuel due to gasification are described by regression of the solid surface. The reduction in solid surface does not impact on the gas motion near the solid surface.

In addition to radiation, flame spread over the solid fuel is influenced by conduction within the fuel and so this mechanism is included within the model. Conduction allows virgin fuel not directly exposed to radiation to be preheated. Generally, heat conduction in solid fuel is considered to be three dimensional. Energy conservation in a solid can be expressed as

$$\frac{\partial \rho_s C_s T_s}{\partial t} = \operatorname{div}(\lambda_s \nabla T_s) \tag{6}$$

where T_s , C_s , ρ_s and λ_s are the temperature, heat capacity, density and thermal conductivity of the solid fuel respectively.

Flame spread over the solid surface represents an interaction between the gas phase combustion and solid phase combustion. This interaction is embodied in the boundary conditions on the interface between gas and solid:

a) in virgin fuel region

$$T = T_{s} \tag{7}$$

$$-\lambda \frac{\partial T}{\partial n} = -\lambda_s \frac{\partial T_s}{\partial n} + \dot{q}''_{r} - \dot{q}'''_{r}$$
(8)

b) in pyrolysis region

$$T = T_s = T_p \tag{9}$$

$$-\lambda \frac{\partial T}{\partial n} = -\lambda_s \frac{\partial T_s}{\partial n} + \dot{q}''_{,-} - \dot{q}''_{,-} - \dot{m}'' L$$
(10)

$$\rho D \frac{\partial m_f}{\partial n} = \dot{m}^{"} (m_f - 1) \tag{11}$$

$$\rho D \frac{\partial m_o}{\partial n} = \dot{m}^{"} m_o \tag{12}$$

where n is the outward going unit normal direction to the solid surface, λ , D, ρ , m_f , m_o are the thermal conductivity, diffusion coefficient, density, fuel mass fraction and oxidant mass fraction in gas phase respectively, and \dot{q}_r^n , \dot{q}_r^n are the radiative heat flux and reradiation losses at the solid surface respectively.

In the simulations presented here, the following solid fuel properties are assumed, $\rho_s = 600.0 \text{ kg/m}^3$, $c_s = 2678.0 \text{ J/(kgK)}$, $\lambda_s = 0.1 \text{ W/(mK)}$, $T_p = 666.0 \text{ K}$. These correspond to the material properties of plywood.

APPLICATIONS

In this section we demonstrate the coupled gaseous/solid phase combustion model through twodimensional simulations of flaming combustion in a room fire scenario involving a plywood ceiling. As two-dimensional simulations are presented here, the four flux radiation model which is a twodimensional version of six flux model is used rather than the latter described above.

The target fuel lining the ceiling is discretised into a number of layers running parallel to the floor. Only the layers directly exposed to the hot fire gases receive the radiative heat fluxes. However, heat is also propagated through the solid material by conduction. Once a layer of the solid fuel is heated to the pyrolysis temperature T_p , it begins to be gasified while its temperature remains fixed at T_p . As it is being gasified, the solid fuel is consumed one layer at time. Once the lining materials have been gasified, the gaseous combustion model (eddy dissipation model) is activated to simulate the flame spread process. For simplicity the gaseous specific heat and molecular weight are assumed to be constants. The radiative heat flux from the fire and hot gases and reradiated heat losses from the solid surface are calculated using the four flux radiation model where the scattering coefficient assumes the value $0.01 \mathrm{m}^{-1}$.

The first case considers an open room scenario in which a flashover type phenomenon is predicted to occur. The second case considers a sealed room fire scenario in which the closed door is opened after some time. In this simulation a backdraft type phenomenon is predicted to occur.

Case 1: Flame Spread Under Lined Ceiling -- Open compartment.

In order to demonstrate the combined solid/gaseous fuel combustion model the following simulation was restricted to two-dimensions. The simulation concerns a two-dimensional compartment measuring 3.6m in length and 2.4m in height and a non-uniform computational mesh consisting of 52×23 (1196) cells is used to discritise the flow domain. In this scenario, a 2.0m high door is open throughout the simulation. The solution domain is extended outside the compartment where the boundary conditions are set as fixed pressure conditions thus allowing fresh air to flow in and combustion products out of the solution domain.

The target solid fuel is located on the ceiling and consists of a 12mm thick cellulosic lining material which covers the entire expanse of the ceiling. This was originally discretised using 1000 cells to model the thickness of the material. A mesh sensitivity study suggested that this could be reduced to 60 cells without a significant loss of accuracy. Finally a mesh of 47×60 cells is used to discretise the solid material. Where the solid fuel has been totally consumed an adiabatic wall boundary condition is imposed.

A source of heat is artificially introduced into the calculation. This is achieved through the introduction of a 100 kW heat source located on the floor adjacent to the back wall. This is active throughout the simulation. It not only provides a heat source for initiating the fire spread along the solid fuel lining the ceiling, but also generates a gas flow to aid the fire spread.

Run on a SUN SPARC 20/612 (with two 60 Mhz processors) system, 100 seconds of simulation requires approximately 2.5 hours of computer time.

Case 2: Flame Spread Under Lined Ceiling -- Sealed compartment

The compartment geometry used in this case is identical to that of case 1. However, in this case the door to the compartment is initially closed and at some point in the simulation it is suddenly opened (door opens completely in one second). As in the previous calculation a 100 kW heat source is located on the floor adjacent to the back wall. However, unlike the previous case, its heat output is gradually reduced, reaching a value of zero when the fire spread in the ceiling material has reached a self sustaining level. After this point the heat source is not reactivated. Eventually, combustion of the pyrolysis products in the room atmosphere diminishes. Several seconds after the model predicts the gaseous combustion to nearly cease, the door to the compartment is opened, allowing fresh oxygen rich air to enter the room.

RESULTS AND DISCUSSION

Case 1: Fire Spread Under Lined Ceiling -- "Flashover"

In order to provide a basis for comparison, first consider the results generated by the model without the solid fuel combustion component. This model simply involves the burner represented as a heat source with constant heat release rate and is equivalent to the simplest form of fire field model used in practice. This case reaches a steady-state after about 100 seconds and produces a maximum hot layer temperature of about 700K. The temperature distribution is similar to the situation shown in figure 2 after 100 seconds.

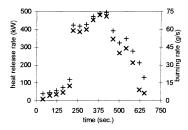


Figure 1: Heat release rate of gaseous combustion and burning rate of solid material in case 1.

+: the heat release rate of gaseous combustion (kW); ×: the burning rate of solid material (g/s).

With the solid fuel combustion model and reactive ceiling included, the situation is very different. The fire development within the compartment appears to undergo a three stage development. This can most clearly be seen in figure 1 which depicts the heat release rate due to gaseous combustion and the burning rate of solid fuel within the compartment.

The curves are clearly divided into three regions representing three phases of fire development. In the first phase, which lasts for the first 200 seconds, the heat release rate of gaseous combustion in the compartment increases at a slow and fairly constant rate. During this phase the lining material is ignited and initially the fire spreads very slowly as there is a backward circulation of gases opposing the spread of hot combustion gases near the junction of the back wall and the ceiling. As the fire progresses, the hot combustion gases break out of this region and more of the ceiling material becomes involved in the combustion (see figure 2 at t = 150s). As the door soffit blocks the flow of hot gases from spilling directly out of the compartment, hot gases begin to accumulate beneath the ceiling forming a stable layer (see figure 2 at t = 150s). This layer preheats the unburned materials and aids the fires progress.

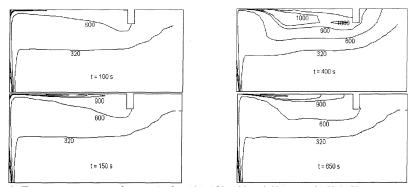
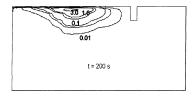


Figure 2: Temperature contours for case 1 after 100, 150, 400 and 650 seconds. Unit: K.



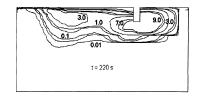


Figure 3: Contours of the heat release rate of gaseous combustion for case 1 preflashover (t = 200s) and during flashover (t = 220s). Unit: kW.

At about 220 seconds (see figure 1) a critical point is reached where the fire rapidly passes into the second phase of fire development and the heat release rate of gaseous combustion in the compartment undergoes a sharp increase(see figures 1 and 3). This rapid increase is a result of the entire combustible ceiling becoming involved in the fire. As a result, the flame erupts out of the compartment (see figure 3 at t = 220s), a phenomena often observed in experiments in which flashover occurs. During flashover, combustion within the gaseous phase is more pronounced and involves a greater proportion of the compartment than is observed during the preflashover stage (see figure 3). Over the next period of about 200 seconds the heat release rate of gaseous combustion and the burning rate reach a maximum and maintain a reasonably stable state. The fire is fully developed in this period (see figure 2 at t = 400s). During this phase the gas temperature beneath the ceiling reaches a peak of about 1100K.

The third phase of fire development occurs approximately after 460 seconds, where the heat release rate begins to rapidly decrease (see figure 1). During this phase all of the remaining solid fuel is consumed, however the heat source driving the flow remains (see figure 2 at t = 650s).

From figure 1 we note that during the first phase of fire development, the burning rate is less than 15 g/s, this rapidly increases to approximately 68 g/s during the second phase, remains approximately constant for a period before entering the third and final phase where it decreases as the fire begins to decline. This result is consistent with a general principle suggested by several experiments[25,26] that there is a limiting burning rate which must be exceeded for a flashover occurrence.

In real enclosure fires, three phases of fire development generally occur:

- a) growth stage, in which the local fire grows smoothly, the end of this phase is usually followed by flashover which is marked by a sharp increase in fire growth rate;
- b) fully developed stage, in which all combustible materials are involved in combustion, this is marked by a period of almost steady burning, and finally,
- c) decay stage, in which the fire begins a rapid decline having consumed most of the fuel.

While the submodels described here are limited by a simple treatment of radiation and an equally simple treatment of gaseous and solid combustion, behaviour similar to this is predicted to occur.

Case 2: Fire Spread Under Lined Ceiling -- "Backdraft"

When the door to the fire compartment is closed, the initial increase in room temperature and ceiling fire spread are more rapid than those noted in case 1. As the door is closed, there is no source of fresh air - and hence oxygen - to replenish the oxygen consumed by the combustion. In this case, while the pyrolysis process continues, combustion is incomplete and more and more

unburned fuel gases accumulate within the room (see figure 4). Figure 4 depicts curves for the heat release rate due to gaseous combustion and the amount of combustible fire products accumulating within the compartment.

Compared with case 1, instead of a sharp increase in heat release rate as the fire spreads, the heat release rate increases slowly however there is a rapid increase in the amount of fuel accumulating within the compartment (see figure 4). After approximately 45 seconds, the heat release rate due to flaming combustion begins to decrease due to the reduction in oxygen concentration. Figure 4 suggests that even as the fire dies down, the amount of fuel accumulating in the compartment continues to increase. This suggests that the pyrolysis process continues as the hot gas mixture provides sufficient energy for the endothermic process to continue.

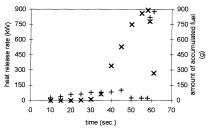


Figure 4: Heat release rate of gaseous combustion and amount of fuel accumulating within the compartment for case 2. +: heat release rate of gaseous combustion (kW); ×: amount of fuel accumulating within the compartment (g).

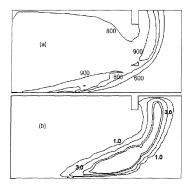


Figure 5: Contours of temperature and heat release rate of gaseous combustion for case 2 at one second after the door is opened. (a): temperature contours (unit: K); (b) heat release rate contours (unit: kW).

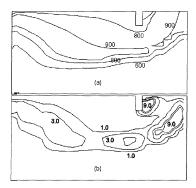


Figure 6: Contours of temperature and heat release rate of gaseous combustion for case 2 at three seconds after the door is opened. (a): temperature contours (unit: K); (b) heat release rate contours (unit: kW).

After 59 seconds, the door of the compartment is opened suddenly. Oxygen rich air is entrained into the room through the lower reaches of the door while the hot fuel rich gas mixture flows out

the room through the upper reaches of the door, under the soffit (see figure 5a). Almost immediately, this motion of hot fuel rich gases and cool oxygen rich air reignites the combustion process (see figure 5b). Figure 5b suggests that initially (i.e. one second after the door is opened), gaseous combustion primarily takes place in the upper layer outside the room, in the doorway and in the lower layer just inside the room. This is due to the nature of the mixing process between the hot fuel rich gases leaving the room and the fresh oxygen rich air entering the room. As a great amount of fuel has accumulated within the compartment (see figure 4), the gaseous combustion is tremendously intense. Furthermore, considerable amounts of combustible gases spill out from the top region of the doorway in a very short space of time generating a large combustion region outside the compartment i.e. the flame protrudes from the compartment (see figure 6). As oxygen rich air mixes with the fuel rich combustion products within the room, flaming combustion erupts through a greater proportion of the compartment in a matter of seconds (see figure 6). These processes result in the marked rapid drop in combustion gases noted in figure 4.

This type of behaviour is similar in nature to the hazardous phenomenon known as backdraft[27,28]. If there is insufficient oxygen to allow flaming combustion to continue, or flashover to occur, the fire will be throttled back and vitiated burning may develop. This is extremely hazardous, for while flaming combustion may be greatly reduced, pyrolysis of the fuel will continue to produce combustible gases within the hot compartment. A sudden in rush of fresh air created by for example, the opening of a door or breaking of a window by a fire fighter, may cause the room to erupt into flame with large flames emerging from the opening posing a significant threat to firefighters[27]. This process is known as backdraft.

As in the previous example, while the submodels described here are limited by a simple treatment of radiation and an equally simple treatment of gaseous and solid combustion, the behaviour exhibited by this model is similar to the highly transient behaviour observed in real backdraft cases. Consider for example the series of scale experiments conducted by Fleischmann et al[28]. While these experiments involve a different scenario and mechanism of reignition to that described in the above numerical simulation, the nature of the backdraft observed in both cases shares several common features, namely:

- a) the reignited flame burns along the front of entrained air;
- b) sizeable flames are observed to emerge from the fire compartment due to the motion of the combustible gases as they escape through the open door;
- c) flames emerge from within the compartment in an extremely short period of time approximately two seconds from the opening of the compartment in both the experiments and the presented numerical predictions;
- d) once the door to the compartment is opened, there is a rapid drop in the amount of combustible fire products accumulated within the compartment.

CONCLUSIONS

A simple solid fuel combustion model consisting of a thermal pyrolysis model, a six flux radiation model and an eddy-dissipation model for gaseous combustion has been implemented within the CFD code CFDS-FLOW3D (version 2.3.3). The model was used to simulate the fire development within a room in which the ceiling - lined with plywood - was the only source of combustible fuel. In the case

of the open compartment fire scenario, the model was able to qualitatively predict behaviour similar to the three stages of fire development - growth and flashover, fully developed and decay. The model was also able to predict the occurrence of a backdraft type phenomenon within a compartment which was originally closed. In this case the model predicted the initial fire growth period, the throttling back of the combustion process and the resulting deflagration when a new opening was suddenly created.

While the pyrolysis model adopted here appears to provide a promising approach to the prediction of fire spread within enclosures, much work remains before it can be applied to engineering applications of fire field modelling. The models reliance on simple treatments of radiation, pyrolysis and gaseous combustion must be assessed. The model must also be demonstrated in three dimensional applications, physical behaviour such as charring and downward flame spread must be included and its suitability for other fuels must be established. Furthermore, quantitative validation of the model with experimental data must be performed. Work along these lines is currently under way.

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