

Improved Radiation and Combustion Routines for a Large Eddy Simulation Fire Model

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ABSTRACT

Improvements have been made to the combustion and radiation routines of a large eddy simulation fire model maintained by the National Institute of Standards and Technology. The combustion is based on a single transport equation for the mixture fraction with state relations that reflect the basic stoichiometry of the reaction. The radiation transport equation is solved using the Finite Volume Method, usually with the gray gas assumption for large scale simulations for which soot is the dominant emitter and absorber. To make the model work for practical fire protection engineering problems, some approximations were made within the new algorithms. These approximations will be discussed and sample calculations presented.

KEY WORDS: finite volume method, large eddy simulation, mixture fraction model

INTRODUCTION

In cooperation with the fire protection engineering community, a large eddy simulation fire model, Fire Dynamics Simulator (FDS), is being developed at NIST to study fire behavior and to evaluate the performance of fire protection systems in buildings. Version 1 of FDS was publicly released in February 2000 [1, 2]. To date, about half of the applications of the model have been for design of smoke handling systems and sprinkler/detector activation studies. The other half consist of residential and industrial fire reconstructions. Throughout its early development, FDS had been aimed primarily at the first set of applications, but following the initial release it became clear that some improvements to the fundamental algorithms were needed to address the second set of applications. The two most obvious needs were for better combustion and radiation models to handle large fires in relatively small spaces, like scenarios involving flashover.

An improved version of FDS, called FDS 2, was released in the fall of 2001. The low Mach number Navier-Stokes equations of FDS version 1 and their numerical solution based on large eddy simulation generally remain the same in FDS 2. What is different are the com-

bustion and radiation routines. FDS 1 contains a relatively simple combustion model that utilizes “thermal elements,” massless particles that are convected with the flow and release heat at a specified rate. While this model is easy to implement and relatively cheap computationally, it lacks the necessary physics to accommodate underventilated fires. A method that handles oxygen consumption more naturally includes an equation for a conserved scalar quantity, known as the mixture fraction, that tracks the fuel and product gases through the entire combustion process. The model assumes that the reaction of fuel and oxygen is infinitely fast, an appropriate assumption given the limited resolvable length and time scales of most practical simulations.

Radiation transport in FDS version 1 was based on a simple algorithm whereby a prescribed fraction of the fire’s energy was distributed on surrounding walls according to a point source approximation. The fire itself was idealized as a discrete set of Lagrangian particles, referred to as “thermal elements,” that released convective and radiative energy onto the numerical grid. This method had two major problems. The first was that only the fire itself radiated; there was no wall to wall or gas to gas radiative heat transfer. Second, the method became expensive when the fire began to occupy a large fraction of the space. A better method for handling radiative heat transfer is to return to the fundamental radiation transport equation for a non-scattering gray gas. The equation is solved using techniques similar to those for convective transport in finite volume methods for fluid flow, thus the name given to it is the Finite Volume Method (FVM).

The new combustion and radiation routines allow for calculations in which the fire itself and the thermal insult to nearby objects can be studied in more detail than before when the fire was merely a point source of heat and smoke. Studies have been performed to examine in detail small scale experiments like the cone calorimeter [3], and fundamental fire scenarios like pool fires [4, 5] and small compartment fires [6]. These calculations are finely resolved, with grid cells ranging from a few millimeters to a few centimeters. However, the majority of model users are still interested mainly in smoke and heat transport in increasingly complex spaces. The challenge to the model developers is to serve both the researchers and practitioners with a tool that contains the appropriate level of fire physics for the problem at hand. This paper describes how the model was improved to better describe the combustion and radiation phenomena, while at the same time maintain its robust hydrodynamic transport routines to handle large scale smoke movement problems.

COMBUSTION

The simplest combustion model that includes the basic stoichiometry of the reaction assumes that the fuel, the oxygen, and the combustion products can be related to a single conserved quantity called the mixture fraction. The obvious advantage of the mixture fraction approach is that all of the species transport equations are combined into one, reducing the computational cost. The mixture fraction combustion model is based on the assumption that large scale convective and radiative transport phenomena can be simulated directly, but physical processes occurring at small length and time scales must be represented in an approximate manner. In short, the model adopted here is based on the assumption that the combustion occurs much more rapidly than the resolvable convective and diffusive phe-

nomena. These same assumptions were made in FDS version 1, where Lagrangian particles known as “thermal elements” were used to represent small packets of unburned fuel. The problem with this idea was that the elements were pre-programmed to release their energy in a given amount of time; the time being derived from flame height correlations of well-ventilated fires. The method broke down when the fire became under-ventilated, or even if the fire was pushed up against a wall [4].

The mixture fraction, Z , is a conserved quantity representing the fraction of gas at a given point that was originally fuel. The mass fractions of all of the major reactants and products can be derived from the mixture fraction by means of “state relations,” empirical expressions arrived at by a combination of simplified analysis and measurement. Start with a general reaction between a fuel and oxygen:



The numbers ν_O , ν_F and ν_P are the stoichiometric coefficients for the overall combustion process that reacts fuel “F” with oxygen “O” to produce a number of products “P”. The stoichiometric equation (1) implies that the mass consumption rates for fuel, \dot{m}_F''' , and oxidizer, \dot{m}_O''' , are related as follows:

$$\frac{\dot{m}_F'''}{\nu_F M_F} = \frac{\dot{m}_O'''}{\nu_O M_O} \quad (2)$$

Under these assumptions, the mixture fraction Z is defined as:

$$Z = \frac{s Y_F - (Y_O - Y_O^\infty)}{s Y_F^I + Y_O^\infty} \quad ; \quad s = \frac{\nu_O M_O}{\nu_F M_F} \quad (3)$$

By design, it varies from $Z = 1$ in a region containing only fuel to $Z = 0$ where the oxygen mass fraction takes on its undepleted ambient value, Y_O^∞ . Note that Y_F^I is the fraction of fuel in the fuel stream. The quantities M_F , M_O , ν_F and ν_O are the fuel and oxygen molecular weights and stoichiometric coefficients, respectively. The mixture fraction Z satisfies the conservation law

$$\frac{\partial \rho Z}{\partial t} + \nabla \cdot \rho \mathbf{u} Z = \nabla \cdot \rho D \nabla Z \quad (4)$$

where ρ is the gas density, D is the material diffusivity, and \mathbf{u} is the flow velocity. Equation (4) is a linear combination of the fuel and oxygen mass conservation equations. The assumption that the chemistry is “fast” means that the reaction that consumes fuel and oxygen occurs so rapidly that the fuel and oxygen cannot co-exist. The interface between fuel and oxygen is the “flame sheet” defined by

$$Z(\mathbf{x}, t) = Z_f \quad ; \quad Z_f = \frac{Y_O^\infty}{s Y_F^I + Y_O^\infty} \quad (5)$$

Because the mixture fraction is a linear combination of fuel and oxygen, additional information is needed to extract the mass fractions of the major species from the mixture fraction. This information comes in the form of “state relations.” Relations for the major components of a simple one-step hydrocarbon reaction are given in Fig. 1.

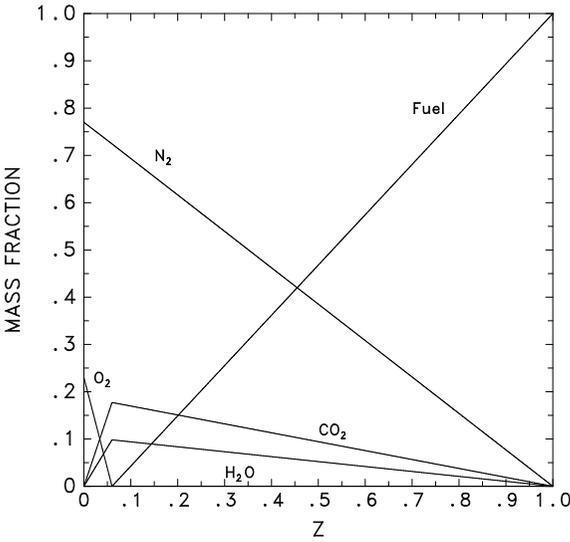


FIGURE 1: State relations for propane.

An expression for the local heat release rate can be derived from the conservation equation for the mixture fraction and the state relation for oxygen. The starting point is Huggett's relationship for the heat release rate as a function of the oxygen consumption rate

$$\dot{q}''' = \Delta H_O \dot{m}'''_O \quad (6)$$

Here, ΔH_O is the heat release rate per unit mass of oxygen consumed, an input parameter to the model that is usually on the order of 13,000 kJ/kg [7]. Equation (6) is the basis for oxygen-consumption calorimetry, and it is consistent with the assumption of infinite-rate kinetics. The oxygen mass conservation equation

$$\rho \frac{DY_O}{Dt} = \nabla \cdot \rho D \nabla Y_O + \dot{m}'''_O \quad (7)$$

can be transformed into an expression for the local heat release rate using the conservation equation for the mixture fraction (4) and the state relation for oxygen $Y_O(Z)$.

$$-\dot{m}'''_O = \nabla \cdot \left(\rho D \frac{dY_O}{dZ} \nabla Z \right) - \frac{dY_O}{dZ} \nabla \cdot \rho D \nabla Z = \rho D \frac{d^2 Y_O}{dZ^2} |\nabla Z|^2 \quad (8)$$

Neither of these expressions for the local oxygen consumption rate is particularly convenient to apply numerically because of the discontinuity of the derivative of $Y_O(Z)$ at $Z = Z_f$ for the ideal state relations. However, an expression for the oxygen consumption rate per unit area of flame sheet can be derived from Eq. (8)

$$-\dot{m}''_O = \left. \frac{dY_O}{dZ} \right|_{Z < Z_f} \rho D \nabla Z \cdot \mathbf{n} \quad (9)$$

In the numerical algorithm, the local heat release rate is computed by first locating the flame sheet, then computing the local heat release rate per unit area, and finally distributing

this energy to the grid cells cut by the flame sheet. In this way, the ideal, infinitesimally thin flame sheet is smeared out over the width of a grid cell, consistent with all other gas phase quantities.

RADIATION

Version 1 of FDS had a simple radiation transport algorithm that used randomly chosen rays from energy-carrying Lagrangian particles to walls and other solid obstructions. This method has two major problems. The first is that only the fire itself radiates; there is no wall to wall or gas to gas radiative heat transfer. Second, the method becomes expensive when the fire begins to occupy a large fraction of the space. A better method for handling radiative heat transfer is to consider the Radiative Transport Equation (RTE) for a non-scattering gas

$$\mathbf{s} \cdot \nabla I_{\lambda}(\mathbf{x}, \mathbf{s}) = \kappa(\mathbf{x}, \lambda) [I_b(\mathbf{x}) - I(\mathbf{x}, \mathbf{s})] \quad (10)$$

where $I_{\lambda}(\mathbf{x}, \mathbf{s})$ is the radiation intensity at wavelength λ , $I_b(\mathbf{x})$ is the source term given by the Planck function, \mathbf{s} is the unit normal direction vector and $\kappa(\mathbf{x}, \lambda)$ is the absorption coefficient at a point \mathbf{x} for wavelength λ .

For practical simulations, the spectral dependence cannot be resolved accurately. Instead, the radiation spectrum can be divided into a relatively small number of bands, and a separate RTE derived for each one [3]. However, even with a small number of bands, the solution of the RTEs is very time consuming. Fortunately, in most large scale fire scenarios soot is the most important combustion product controlling thermal radiation from the fire and hot smoke. Because the radiation energy is distributed over a wide range of wavelengths under these circumstances, it is convenient to assume that the gas behaves as a gray medium. The spectral dependence is lumped into one absorption coefficient and the source term is given by the blackbody radiation intensity

$$I_b(\mathbf{x}) = \sigma T(\mathbf{x})^4 / \pi \quad (11)$$

In optically thin flames, where the amount of soot is small compared to the amount of CO₂ and water, the gray gas assumption may produce significant over-predictions of the emitted radiation, in which case the multi-band radiation model is needed.

For the calculation of the gray (and if necessary band) mean absorption coefficients κ (κ_n), a narrow-band model, RadCal [8], is combined with FDS. At the beginning of a simulation, the absorption coefficients are tabulated as a function of mixture fraction and temperature. During the simulation the local absorption coefficient is found from a pre-computed table. An important consideration in computing the entries in the table is the fact that the radiation spectrum is dependent on a path length due to the widening and overlapping of the individual lines. Thus the “effective” absorption coefficient will be a function of the distance over which the line-of-sight form of the RTE is integrated. In FDS, a fraction of the characteristic length of the computational domain is chosen as the path length used by RadCal in computing effective gray gas absorption coefficients. A proper definition of path length in the context of band mean absorption coefficients is still a subject of active research.

In calculations of limited spatial resolution, the source term, I_b , in the RTE requires special

treatment in the neighborhood of the flame sheet because the temperature is smeared out over a grid cell and thus is considerably lower than one would expect in a diffusion flame if the cell is relatively large. Moreover, the soot volume fraction within the flame itself is not known in the calculation. Even if it were, it would be difficult to model its effect on the emission of thermal radiation when using a coarse grid. All that is usually known about a given fuel is how much of its mass is converted into soot and transported away from the fire. Because of its dependence on the soot volume fraction and on the temperature raised to fourth power, the source term in the RTE must be modeled in those grid cells cut by the flame sheet. Away from the flame, where the temperatures are lower, greater confidence in the computed temperature and soot volume fraction permits the source term to take on its traditional value. Thus, in FDS a decision is made when computing the source term in the RTE based on whether combustion is occurring in a given grid cell

$$\kappa I_b = \begin{cases} \kappa \sigma T^4 / \pi & \text{Outside flame zone} \\ \chi_r \dot{q}''' / 4\pi & \text{Inside flame zone} \end{cases} \quad (12)$$

where \dot{q}''' is the chemical heat release rate per unit volume and χ_r is the *local* fraction of that energy emitted as thermal radiation. Note the difference between the prescription of a local χ_r and the resulting global equivalent. For small fires ($D < 1$ m), the local χ_r is approximately equal to its global counterpart, however, as the fires increase in size, the global value will typically decrease due to a net re-absorption of the thermal radiation by the increasing smoke mantle [9].

LARGE SCALE FIRE SIMULATIONS

To date, the new combustion and radiation solvers have been applied to a wide variety of fire problems to assess the cost, robustness and accuracy of the new routines. One of the first concerns for both sub-models was their cost. The mixture fraction combustion algorithm requires the solution of an additional transport equation for Z , adding about 20 % to the overall CPU time. The radiation routine could cost an unacceptably high amount if the gray gas assumption was not applied, and if the entire RTE were solved every time step. Since radiation accounts for about 35 % of the energy transport in a typical fire scenario, it was decided that no more than 35 % of the CPU time ought to be devoted to the radiation transport. As a cost-saving measure, the gray RTE equation is solved gradually over approximately 15 time steps. Every 3 time steps 1/5 of the approximately 100 solid angle equations are updated, and the results stored as running averages. Although the code user can control these parameters, it has been found that with the given defaults, the finite volume solver requires 15 % to 20 % of the total CPU time of a calculation, a modest cost given the complexity of radiation heat transfer.

A calculation is presented here that are typical of the type of fire scenario that the model has been re-designed to address. A snapshot from the FDS visualization package Smokeview is shown in Fig. 2. A small cushion is ignited on a couch in a room that is roughly 5 m by 5 m by 2.5 m with a single door leading out. The fire grows to the point of flashover in about 3 min. This simulation is based on an experiment performed by the University of Maryland and the Bureau of Alcohol, Tobacco and Firearms.

The new combustion and radiation routines are crucial to this calculation because towards

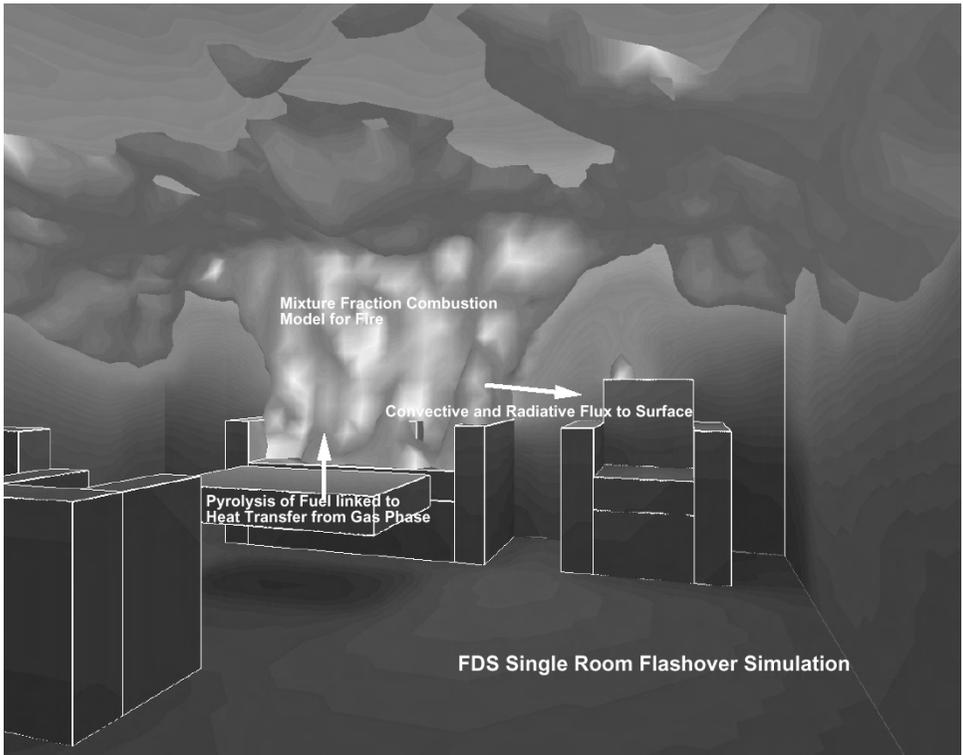


FIGURE 2: Sample simulation of a room fire using the new combustion and radiation routines. Shown is the flame sheet where the mixture fraction is at its stoichiometric value.

flashover and beyond, the room conditions are severely underventilated and radiation is the dominant mode of heat transfer. The gray gas assumption is made because the radiation is dominated by soot, and because the relative coarseness of the numerical grid (10 cm) does not justify the expense of the multi-band radiation model. The fuel consists of polyurethane, wood, and a variety of fabrics whose thermal properties are known only in the most general sense. The soot volume fraction is based solely on estimates of the smoke production; the actual values within the flames are unknown. In generating effective absorption coefficients with RadCal, it is assumed that the fuel is methane. Clearly more research is needed to fill in many of the missing pieces. Refinement of the numerical algorithm and comparison with experiment is ongoing.

GRID DEPENDENCE

During a period of about a year when the combustion and radiation models were being implemented and tested, the effect of the numerical grid on the results was a major concern. Now that the emphasis had shifted from smoke movement away from the fire to heat transfer in the immediate vicinity of the fire, the size of the numerical grid cells became

more important. In many calculations that involve either relatively large spaces or relatively small fires, the grid resolution in the vicinity of the fire will be severely limited. For many applications, this in itself may not be a problem since the fire merely serves as a point source of heat and smoke. However, if one is interested in flame spread, near-field heat transfer is all-important, and the resolution of the numerical grid, especially during the early stage of a fire, cannot be ignored.

We have found from various validation exercises involving pool fires and small compartments that good agreement with experimental data is possible when the fire is adequately resolved. However, even in cases where the fire is not well-resolved, it is possible to get a reasonable approximation of the total and radiative heat release rate of the fire, plus its volumetric distribution and flame height, with numerical grids that are very coarse. To do this, one needs to slightly modify the procedure for obtaining the local heat release rate from the mixture fraction field. Note that this approximation is only intended for under-resolved fires. The above procedure for determining the local heat release rate works well for calculations in which the fire is adequately resolved.

What do we mean by “adequately resolved”? It depends on what the objective of the calculation is. To a chemical kineticist, adequate resolution might involve micrometers and microseconds; to a fire dynamicist, millimeters and milliseconds; to a fire protection engineer, meters and seconds. A *relative* measure of how well a fire is resolved numerically is given by the nondimensional expression $D^*/\delta x$, where D^* is a characteristic fire diameter

$$D^* = \left(\frac{\dot{Q}}{\rho_\infty c_p T_\infty \sqrt{g}} \right)^{\frac{2}{5}} \quad (13)$$

and δx is the nominal size of a grid cell. Note that the characteristic fire diameter is related to the characteristic fire size via the relation $\dot{Q}^* = (D^*/D)^{5/2}$, where D is the physical diameter of the fire. The quantity $D^*/\delta x$ can be thought of as the number of computational cells spanning the characteristic (not necessarily the physical) diameter of the fire. The more cells spanning the fire, the better the resolution of the calculation. For fire scenarios where D^* is small relative to the physical diameter of the fire, and/or the numerical grid is relatively coarse, the stoichiometric surface $Z = Z_f$ will underestimate the observed flame height [4]. It has been found empirically that a good estimate of flame height can be found for crude grids if a different value of Z is used to define the combustion region

$$\frac{Z_{f,\text{eff}}}{Z_f} = \min \left(1, C \frac{D^*}{\delta x} \right) \quad (14)$$

Here C is an empirical constant to be used for all fire scenarios. As the resolution of the calculation increases, the $Z_{f,\text{eff}}$ approaches the ideal value, Z_f . The benefit of the expression is that it provides a quantifiable measure of the grid resolution that takes into account not only the size of the grid cells, but also the size of the fire.

A practical consideration when implementing this idea in the numerical model is that in most cases D^* is not known in advance if the fire is allowed to spread throughout a space. Somehow the quantity $D^*/\delta x$ must be approximated based only on values of the fuel mass

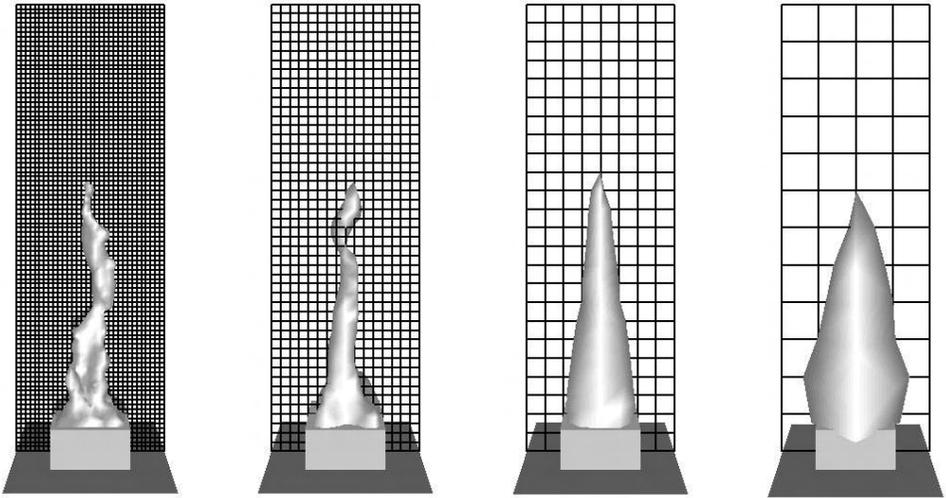


FIGURE 3: Simulations of a 0.4 m by 0.4 m sand burner with progressively coarser resolution; from left to right, 2.5 cm, 5 cm, 10 cm and 20 cm grid cells.

flux, cell size, and mixture fraction near the burning surface. Assuming the actual fire diameter $D \sim n\delta x$ where n is the number of cells spanning the fire, it can be shown after substituting terms that

$$\frac{D^*}{\delta x} \sim n^{4/5} \dot{Q}_{\text{local}}^{*2/5} \quad (15)$$

where \dot{Q}_{local}^* is a quantity that resembles \dot{Q}^* , but it is defined locally

$$\dot{Q}_{\text{local}}^* = \frac{\dot{q}''}{\rho_{\infty} c_p T_{\infty} \sqrt{g \delta x}} \quad (16)$$

The number of cells spanning D^* , n , is not readily obtained in a calculation, but it has been found from numerous trials that n is proportional to the maximum value of Z in the gas phase cells of the numerical grid. In most practical calculations, Z is far less than its ideal value of unity in the first gas phase grid cell above the burner due to the increased numerical diffusion necessitated by the coarse grid.

Figure 3 shows the flame sheet from four simulations of a simple 0.4 m by 0.4 m propane sand burner set to 160 kW. The only difference between each is the grid resolution. Only the case with a 2.5 cm grid cell was run without need of the modified flame surface value. For the 5 cm case, the resolution factor was about 0.7, for the 10 cm case, the factor was 0.3, and for the 20 cm case the factor was about 0.1; all approximate since the factor fluctuates slightly during the calculation. For propane, $Z_f = 0.06$. Since the diffusion coefficient used in the calculation is only of order δx^2 , the flame surface in the 20 cm case would just barely appear above the burner. An other way to look at it is that we are assuming fuel and oxygen burn instantaneously. The mixture fraction combustion model is equivalent to tracking

propane and oxygen through their respective transport equations and never allowing both fuel and oxygen to exist in a single grid cell. As fuel emerges from the burner surface, it will mix with a disproportionately large amount of oxygen in the first grid cell adjacent to the burner. All of the heat of combustion will be liberated in that first grid cell, and the flame height will be under-predicted. This phenomenon was noticed by Ma and Quintiere [4] who were doing some validation exercises involving flame height.

The adjustment of the flame surface is almost always necessary when the simulation starts with a small ignition source. It is usually impractical to provide a fine grid wherever the fire resides, since usually the fire will grow and spread. The benefit of the technique described here is that as the fire grows, D^* grows, and the reliance on the adjusted flame sheet value diminishes, and in many cases goes away entirely. For example, a flashed over room from a numerical point of view is a fire resolved with a numerical grid spanning the length and width of the room. However, during the initial growth stage, the fire may be supported by just a few grid cells spanning the width of the small fire. Of course, there are techniques used in various fields of CFD to apply fine grids to where they are needed, even adjusting the grids during a calculation. This latter technique, adaptive grid refinement, is difficult to apply and increases the cost of the calculation significantly. A more modest technique, known as multi-block, allows the user to specify grids of various refinement throughout the computational domain. Its practical application would be to finely grid a room of origin in a building, and use a coarser grid elsewhere. Such an effort is underway at NIST, but no matter how well it works, there will probably always be a need to model a relatively small fire on a relatively coarse grid.

Figure 4 displays some predicted flame heights versus two experimental correlations. The calculations were performed for a 0.3 m square gas burner with no lip and heat release rates varying from 7 kW to 1,800 kW. For the low Q^* fires, the Cox and Chitty data is appropriate since they used square gas burners in their experiments [10]. The adjustment of the flame surface was used for the cases in which $Q^* < 1$. For all the rest, the flame sheet location was chosen based solely on the ideal stoichiometry. In all cases, a uniform grid was used to simulate the fires, with a cell size of 3.75 cm or 8 cells spanning the burner width. For the larger Q^* fires, the numerical resolution is adequate to capture the gross features of the fire, in particular its flame height. For the low Q^* fires, the flame heights are comparable to the size of a single grid cell, in which case it is not possible to accurately predict the flame height. Even so, the energy from the fire is deposited onto the numerical grid as well as can be expected given the numerical resolution.

CONCLUSION

New combustion and radiation routines have been implemented in a large eddy simulation fire model. With both, we seek to improve the physical models so that we can understand better the dynamics of a fire, but we want the model to remain useful for practicing engineers who have limited computing resources and limited information about the materials burning in a typical fire. Even as we develop more sophisticated numerical algorithms to describe the growth and suppression of fires, many users will still use the model primarily for smoke movement and detector activation in which case only the overall mass, momen-

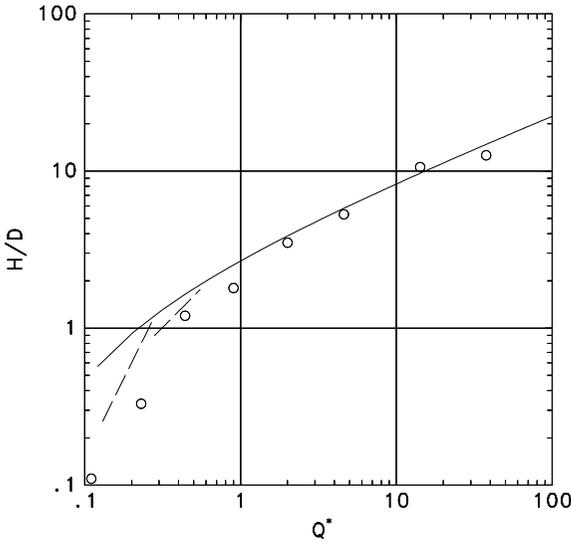


FIGURE 4: Comparison of predicted flame heights versus Hestekstad's correlation (solid line) [11] and Cox and Chitty's (dashed line) [10].

tum and energy transport from the fire is needed. The objective of the model development is to make it as useful as possible for a wide variety of applications, both fundamental and applied. If successful, the model will be exercised by a large variety of users which eliminates computer bugs, introduces field modeling to a new generation of fire protection engineers, and most importantly provides validation of the algorithms for a wide variety of experimental data sets. This is an evolving process. Work still needs to be done in many areas, especially soot production, radiation absorption coefficients, numerical resolution, and material properties. Progress will be made because of better research in the future, but also because of lessons learned from calculations being performed now. The development of zone models over the past few decades certainly benefited from the wide use of the early models, pointing out both the strengths and weaknesses, and ultimately guiding the development of newer algorithms. The same will be true of field models if the proper balance is struck between research and practical application.

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