DEVELOPMENT OF COMBUSTION AND RADIATION MODELS FOR LARGE SCALE FIRE SIMULATON

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INTRODUCTION

In cooperation with the fire protection engineering community, a numerical 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 development, FDS has been aimed primarily at the first set of applications, but it is now clear that some improvements to the fundamental algorithms are needed to address the second set of applications. The two most obvious needs are for better combustion and radiation models to handle large fires in relatively small spaces, like scenarios involving flashover.

Version 1 of FDS 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 more comprehensive method that handles oxygen consumption more naturally solves an equation for a conserved scalar quantity, known as the mixture fraction, which is the fraction of gas at a given point in the flow field that originated as fuel. The model assumes that combustion is mixing-controlled, and that the reaction of fuel and oxygen is infinitely fast. 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.

Version 1 of FDS has a simple radiation transport algorithm that uses randomly chosen rays between radiation sources and targets, a method commonly known as "ray tracing." 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 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). To date, this solver has been im-

plemented in an experimental version of FDS. Using approximately 100 discrete angles, the finite volume solver requires about 15% of the total CPU time of a calculation, a modest cost given the complexity of radiation heat transfer.

IMPROVEMENTS TO THE FIRE DYNAMICS SIMULATOR

The low Mach number Navier-Stokes equations of FDS version 1 and their numerical solution generally remain the same in version 2. What is different is the handling of the source term in the energy conservation equation representing the chemical heat release rate and the redistribution of heat due to thermal radiation. This section briefly discusses the new algorithms.

Combustion

The original version of FDS 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 more comprehensive method that handles oxygen consumption more naturally involves an equation for a conserved scalar quantity, known as the mixture fraction, that represents a linear combination of the fuel and oxygen transport equations. 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 is mixing-controlled. 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.

The mixture fraction Z is defined as:

$$Z = \frac{sY_F - \left(Y_O - Y_O^\infty\right)}{sY_F^I + Y_O^\infty} \quad ; \quad s = \frac{\nu_O M_O}{\nu_F M_F} \tag{1}$$

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

$$\frac{\partial \rho Z}{\partial t} + \nabla \cdot \rho \mathbf{u} Z = \nabla \cdot \rho D \nabla Z \tag{2}$$

where ρ is the gas density, D is the material diffusivity, and $\mathbf{u}$ is the flow velocity. Equation (2) 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"
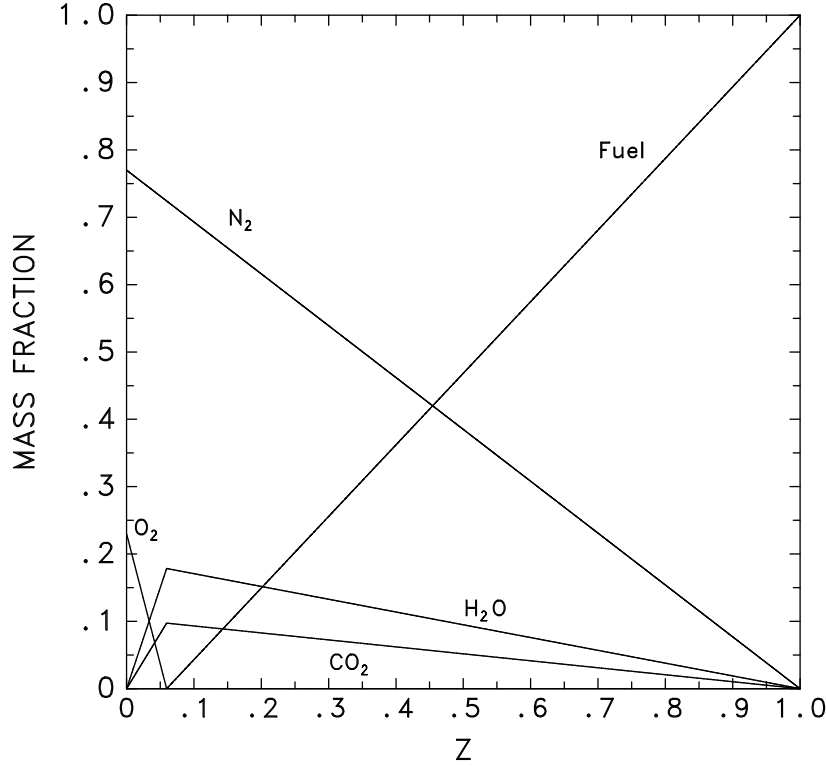
FIGURE 1: State relations for propane.

defined by

$$Z(\mathbf{x},t) = Z_f \quad ; \quad Z_f = \frac{Y_O^\infty}{sY_F^I + Y_O^\infty} \tag{3}$$

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.

An expression for the local heat release rate can be derived from the conservation equations and the state relation for oxygen. The starting point is Huggett's [3] relationship for the heat release rate as a function of the oxygen consumption

$$\dot{q}''' = \Delta H_O \dot{m}_O''' \tag{4}$$

Here, ΔH_O is the heat release rate per unit mass of oxygen consumed, usually on the order of 13,000 kJ/kg for most fuels [3]. The oxygen mass conservation equation

$$\rho \frac{DY_O}{Dt} = \nabla \cdot \rho D \nabla Y_O + \dot{m}_O''' \tag{5}$$

can be transformed into an expression for the local heat release rate using the conservation equation for the mixture fraction (2) and the state relation for oxygen $Y_O(Z)$.

$$-\dot{m}_O''' = \nabla \cdot \left(\rho D \frac{dY_O}{dZ} \nabla Z \right) - \frac{dY_O}{dZ} \nabla \cdot \rho D \nabla Z = \rho D \frac{d^2 Y_O}{dZ^2} |\nabla Z|^2 \tag{6}$$

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 $Z = Z_f$. However, an expression for the oxygen consumption rate per unit area of flame sheet can be derived from Eq. (6)

$$-\dot{m}_O'' = \left.\frac{dY_O}{dZ}\right|_{Z<Z_f} \rho D \, \nabla Z \cdot \mathbf{n} \tag{7}$$

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, infinitessimally 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 has a simple radiation transport algorithm that uses randomly chosen rays between radiation sources and targets, a method commonly known as "ray tracing." 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

$$\mathbf{s} \cdot \nabla I_\lambda(\mathbf{x}, \mathbf{s}) = \kappa(\mathbf{x}, \lambda) \, [I_b(\mathbf{x}) - I(\mathbf{x}, \mathbf{s})] \tag{8}$$

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.

In practical simulations the spectral dependence cannot be solved accurately. However, if the radiation spectrum is divided into a relatively small number of bands, and a separate RTE is solved for each band, a more accurate solution can be obtained. The limits of the bands are selected to give an accurate representation of the most important radiation bands of CO_2 and water. The band specific RTE's are now

$$\mathbf{s} \cdot \nabla I_n(\mathbf{x}, \mathbf{s}) = \kappa_n(\mathbf{x}) \, \left[I_{b,n}(\mathbf{x}) - I(\mathbf{x}, \mathbf{s})\right], \quad n = 1...N \tag{9}$$

where I_n is the intensity integrated over the band n, κ_n is the aproppriate mean absorption coefficient inside the band. The source term can be written as a fraction of the blackbody radiation

$$I_{b,n} = F_n(\lambda_{\min}, \lambda_{\max}) \, \sigma \, T^4 / \pi \tag{10}$$

where σ is the Stefan-Boltzmann constant. The calculation of factors F_n is explained, for example, in [4]. When the intensities corresponding to the bands are known, the total intensity is calculated by summation

$$I(\mathbf{x}, \mathbf{s}) = \sum_{n=1}^{N} I_n(\mathbf{x}, \mathbf{s}) \tag{11}$$

By numerical experiments it was found that six bands are usually enough ($N = 6$). If the absorption of the fuel is known to be important, separate bands should be reserved for fuel, and the total number of bands is ten ($N = 10$). For simplicity, the fuel is assumed to be CH_4. Also, the contribution from CO is small compared to CO_2 and H_2O. The limits of the bands are shown in Table 1.

TABLE 1: Limits of the spectral bands.

CO₂ and H₂O bands										
ν (1/cm)	10000	3800	3450	2400	2200	1000	50			
λ (μm)	1.0000	2.63	2.90	4.17	4.55	10.0	200.0			
CH₄, CO₂ and H₂O bands										
ν (1/cm)	10000	3800	3450	3200	2800	2400	2200	1400	1200	1000	50
λ (μm)	1.00	2.63	2.90	3.13	3.57	4.17	4.55	7.14	8.33	10.0	200.0

Even with a reasonably small number of bands, the solution of N RTE's is very time consuming. Fortunately, in most large scale fire scenarios soot is the most important combustion product affecting thermal radiation from the fire and hot smoke. As the radiation spectrum of soot is continuous, it is then possible to assume that the gas behaves as a gray medium. The spectral dependence is lumped into one absorption coefficient ($N = 1$) and the source term is given by the blackbody radiation intensity

$$I_b(\mathbf{x}) = \sigma T(\mathbf{x})^4 / \pi \qquad (12)$$

In optically thin flames, where the amount of soot is small compared to the amount of CO_2 and water, the gray gas assumption may produce significant overpredictions of the emitted radiation.

For the calculation of the gray and band mean absorption coefficients κ_n, a narrow-band model RADCAL [5] is combined with FDS. In the beginning of the 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.

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 temperatures are smeared out over a grid cell and thus are considerably lower than one would expect in a diffusion flame. Plus, the soot volume fraction within the flame itself is not known, and 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. Elsewhere, there is greater confidence in the computed temperature and soot volume fraction, and the source term can take on its traditional value away from the flame.

$$\kappa I_b = \begin{cases} \kappa \sigma T^4 / \pi & \text{Outside flame zone} \\ \chi_r \dot{q}''' / 4\pi & \text{Inside flame zone} \end{cases} \qquad (13)$$

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 [6].

The boundary condition for the radiation intensity leaving the gray diffuse wall is given as

$$I_w(\mathbf{s}) = \varepsilon I_{bw} + \frac{1 - \varepsilon}{\pi} \int_{\mathbf{s'} \cdot \mathbf{n}_w < 0} I_w(\mathbf{s'}) \, |\mathbf{s'} \cdot \mathbf{n}_w| \, d\Omega \tag{14}$$

where $I_w(\mathbf{s})$ is the intensity at the wall, ε is the wall emissivity, and I_{bw} is the black body intensity at the wall.

The radiative transport equation (9) is solved using techniques similar to those for convective transport in finite volume methods for fluid flow [7], thus the name given to it the Finite Volume Method (FVM). To obtain the discretized form of the RTE, the unit sphere is divided into a finite number of solid angles. In each grid cell a discretized equation is derived by integrating equation (8) over the cell ijk and the control angle $\delta\Omega^l$, to obtain

$$\int_{\Omega^l} \int_{V_{ijk}} \mathbf{s} \cdot \nabla I_n(\mathbf{x}, \mathbf{s}) dV d\Omega = \int_{\Omega^l} \int_{V_{ijk}} \kappa_n(\mathbf{x}) \left[I_{b,n}(\mathbf{x}) - I_n(\mathbf{x}, \mathbf{s}) \right] dV d\Omega \tag{15}$$

The volume integral on the left hand side is replaced by a surface integral over the cell faces using the divergence theorem. Assuming that the radiation intensity $I(\mathbf{x}, \mathbf{s})$ is constant on each of the cell faces, the surface integral can be approximated by a sum over the cell faces.

The radiant heat flux vector $\mathbf{q}_r$ is defined

$$\mathbf{q}_r(\mathbf{x}) = \int \mathbf{s} I(\mathbf{x}, \mathbf{s}) \, d\Omega \tag{16}$$

The radiative loss term in the energy equation is

$$-\nabla \cdot \mathbf{q}_r(\mathbf{x}) = \kappa(\mathbf{x}) \left[U(\mathbf{x}) - 4\pi I_b(\mathbf{x}) \right] \quad ; \quad U(\mathbf{x}) = \int_{4\pi} I(\mathbf{x}, \mathbf{s}) \, d\Omega \tag{17}$$

In words, the net radiant energy gained by a grid cell is the difference between that which is absorbed and that which is emitted.

To date, this solver has been implemented in an experimental version of FDS. Using approximately 100 angles, the finite volume solver requires about 15% of the total CPU time of a calculation, a modest cost given the complexity of radiation heat transfer. Sample calculations are shown in Figs. 2 and 3. 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. In Fig. 3, a house made entirely of wood burns from a fire on the stove. The room fire example is based on an actual experiment performed by the University of Maryland and the Bureau of Alcohol, Tobacco and Firearms. The house fire is entirely fictitious, and meant to serve simply as a demonstration of various features of the model.
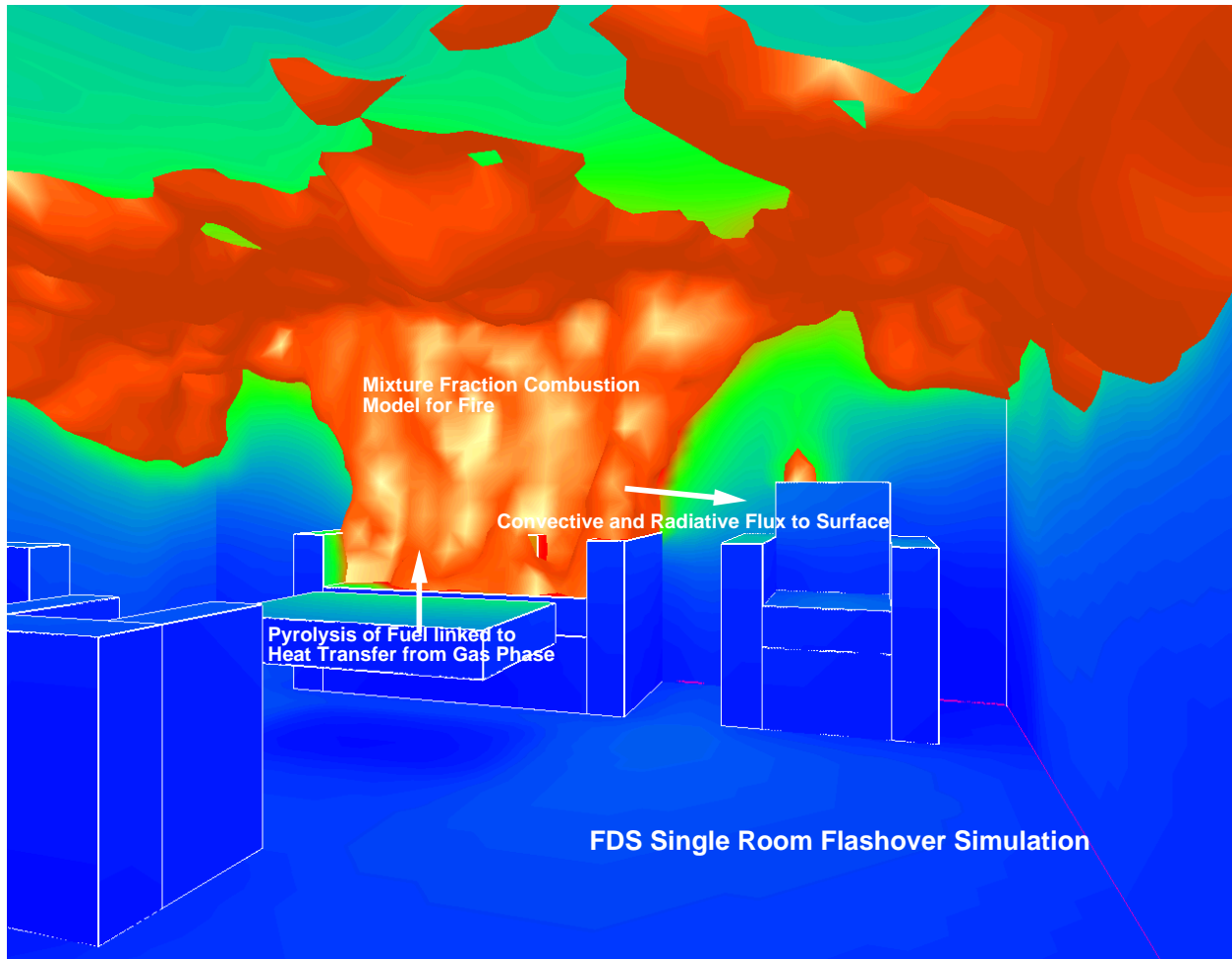
FIGURE 2: Sample simulation of a room fire using the new combustion and radiation routines. Shown is the flame sheet where the mixture fraction is at its stoichiometric value.

The new combustion and radiation routines are crucial to these calculations because towards flashover and beyond, the room conditions are severely underventilated and radiation is the dominant mode of heat transfer. In both examples, 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, 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.
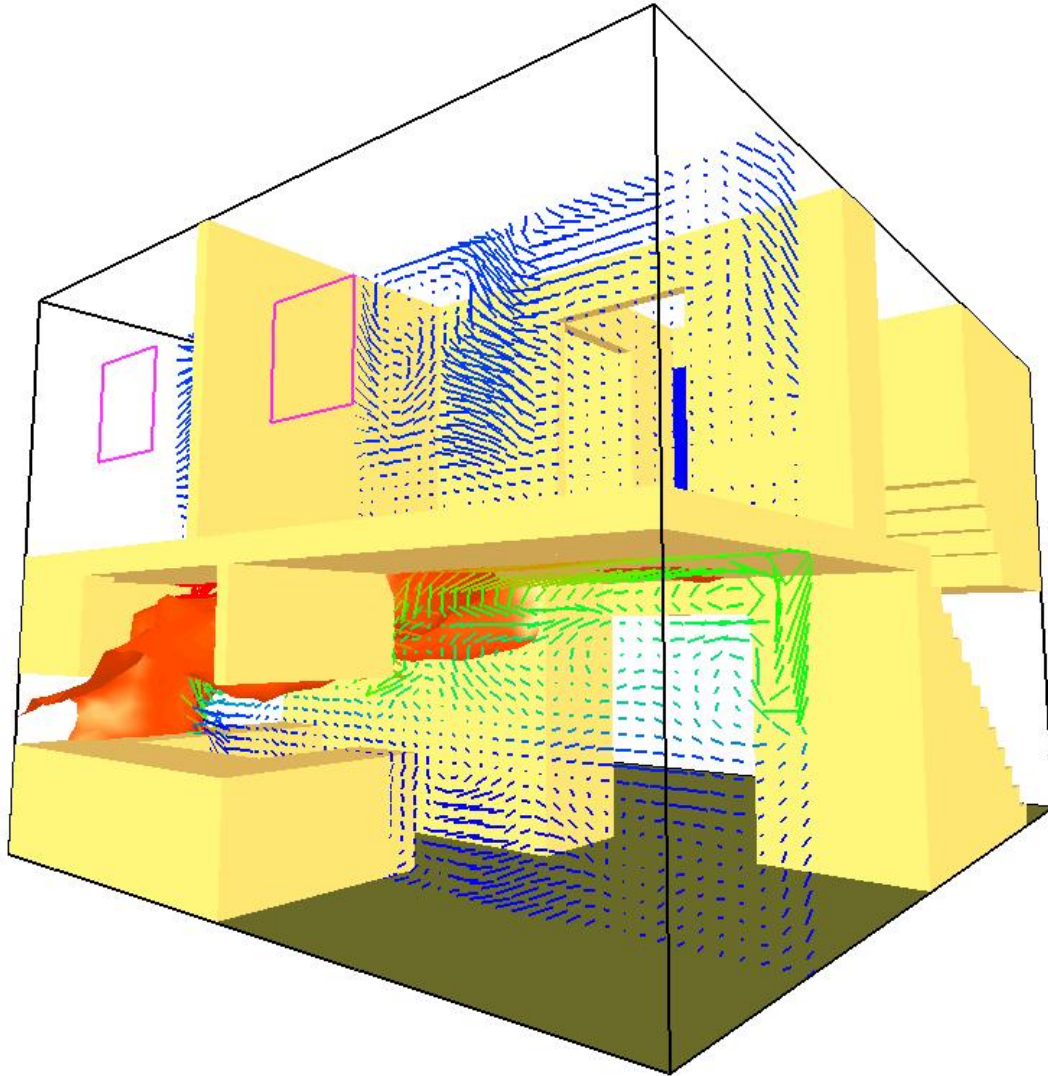
ACKNOWLEDGEMENTS

FIGURE 3: Sample simulation of a house fire using the new combustion and radiation routines. Shown is the flame sheet and a slice of flow vectors.

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