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Large Eddy Simulations of Smoke Movement in Three Dimensions

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Abstract

A methodology for the prediction of smoke movement in enclosures is presented. The method is based on high resolution solutions of the Navier-Stokes equations specialized to the smoke movement problem. Forced ventilation, complex geometry, and water spray effects are incorporated in the model. Sample calculations illustrating the capabilities of this approach are presented, and a comparison of model predictions with room doorway experiments performed by Steckler are shown. The results indicate that the convective transport of smoke and hot gases can be simulated without recourse to empirical models of turbulence.

1 Introduction

This paper describes a methodology for simulating the transport of smoke and hot gases in enclosures. The approach is based on the use of efficient CFD techniques and high performance computers to solve a form of the Navier Stokes equations specialized to the smoke movement problem. The fire is prescribed in a manner consistent with a mixture fraction based approach to combustion, but the combustion phenomena themselves are not simulated. The mixing and transport of smoke and hot gases is calculated directly from an approximate form of the Navier Stokes equations. The computations are carried out as a three dimensional time dependent process, limited only by the spatial resolution of the underlying grid. No turbulence models are employed; the large scale eddies are simulated directly and sub-grid scale motions are suppressed. Present capabilities permit a typical residential room or hotel unit to be simulated at a 3-5 cm. resolution limit. The enclosure can have any shape made up of rectangular blocks, and can be multiply connected. The smoke is simulated by tracking a large number of Lagrangian elements, which originate in the fire. These same elements carry the heat released by the fire, providing a self consistent description of the smoke transport at all resolvable length and time scales. Large temperature and pressure variations are permitted, subject to the limitation that the Mach Number is much less than one. A simulation of the effects of a water sprinkler spray on the smoke movement can also be studied. The following section gives a brief description of the mathematical and computational aspects of the model, while the final section illustrates its capability with sample results and a comparison with experiment. The influence of Prof. Zukoski on the field of smoke movement in general and our work in particular has been profound. It is a pleasure to dedicate this paper to him.

2 Mathematical Model

The Navier Stokes equations are cast in terms of a velocity $\vec{u}$, a modified temperature $\tilde{T}$, density $\tilde{\rho}$, and perturbation pressure $\tilde{p}$. The modified quantities are defined so that the corresponding time dependent spatially averaged thermodynamic quantities $T_0(t)$, $\rho_0(t)$ and $p_0(t)$ are factored out of the equations actually solved on the computer. The spatially averaged quantities play the same role that ambient conditions do in the Boussinesq approximation. The modified variables are related to the physical temperature T, density ρ, and pressure p as follows:

$$\begin{aligned} T &= T_0(t)(1+\tilde{T}(\vec{r},t)) \\ \rho &= \rho_0(t)(1+\tilde{\rho}(\vec{r},t)) \\ p &= p_0(t) - \rho_0(t)gz + \tilde{p}(\vec{r},t) \end{aligned} \quad (1)$$

The spatially averaged quantities are obtained by combining global mass and energy balances with the equation of state and a definition of T_0 in terms of p_0 through an adiabatic process.

$$\frac{T_0(t)}{T_0(0)} = \left(\frac{p_0(t)}{p_0(0)}\right)^{\frac{\gamma-1}{\gamma}} \quad (2)$$

$$p_0 \oint \vec{u}\cdot\vec{n}dS + \frac{V}{\gamma}\frac{dp_0}{dt} = \frac{\gamma-1}{\gamma}(\dot{Q} - \oint q_w dS) \quad (3)$$

$$p_0 = \rho_0 R T_0 \quad (4)$$

Here, $\vec{n}$ is a unit normal pointing out of the enclosure, γ is the specific heat ratio, $\dot{Q}$ is the total heat released into the gas, and q_w the local heat flux from the gas to the wall. The integrals are carried out over all the boundaries of the enclosure. In meteorology, the concept of an effective temperature defined in terms of a background pressure is called a "potential temperature".

The local mass and energy conservation equations can now be combined to yield:

$$\nabla\cdot\vec{u} + \frac{1}{\gamma p_0}\frac{dp_0}{dt} = \alpha_0(t)\nabla\cdot(\tilde{k}\nabla\tilde{T}) + \frac{\gamma-1}{\gamma}\frac{\dot{q}}{p_0} \quad (5)$$

$$(1+\tilde{\rho})\left(\frac{\partial\tilde{T}}{\partial t} + \vec{u}\cdot\tilde{T}\right) = \alpha_0(t)\nabla\cdot(\tilde{k}\nabla\tilde{T}) + \frac{\gamma-1}{\gamma}\frac{\dot{q}}{p_0} \quad (6)$$

The average thermal diffusivity $\alpha_0(t) = k_0(T_0)/\rho_0 c_p$ where the thermal conductivity $k(T)$ is written in the form $k = k_0(T_0)\tilde{k}$. The momentum equation is written in vector invariant form as follows:

$$\frac{\partial\vec{u}}{\partial t} - \vec{u}\times\vec{\omega} + \nabla\mathcal{H} + \tilde{T}\vec{g} - \vec{F} = (1+\tilde{T})\nu_0(t)\nabla\cdot\overleftrightarrow{\tau} \quad (7)$$

$$\mathcal{H} = \frac{\tilde{p}}{\rho_0} + \frac{u^2}{2} \quad (8)$$

$$\begin{aligned} \nabla\cdot\overleftrightarrow{\tau} &= \frac{4}{3}\nabla(\tilde{\mu}\nabla\cdot\vec{u}) + \nabla(\vec{u}\cdot\nabla\tilde{\mu}) - (\nabla^2\tilde{\mu}\vec{u}) + \\ &\quad \nabla\tilde{\mu}\times\vec{\omega} - (\nabla\cdot\vec{u})\nabla\tilde{\mu} - \nabla\times\nabla\times(\tilde{\mu}\vec{u}) \end{aligned} \quad (9)$$

The average kinematic viscosity $\nu_0(t) = \mu_0(T_0)/\rho_0$ where the viscosity $\mu(T)$ is written as $\mu = \mu_0(T_0)\tilde{\mu}$. The quantity $\vec{\omega} = \nabla\times\vec{u}$ is the vorticity. The quantity $\vec{F}$ is the droplet drag density transferred to the gas by the water spray.

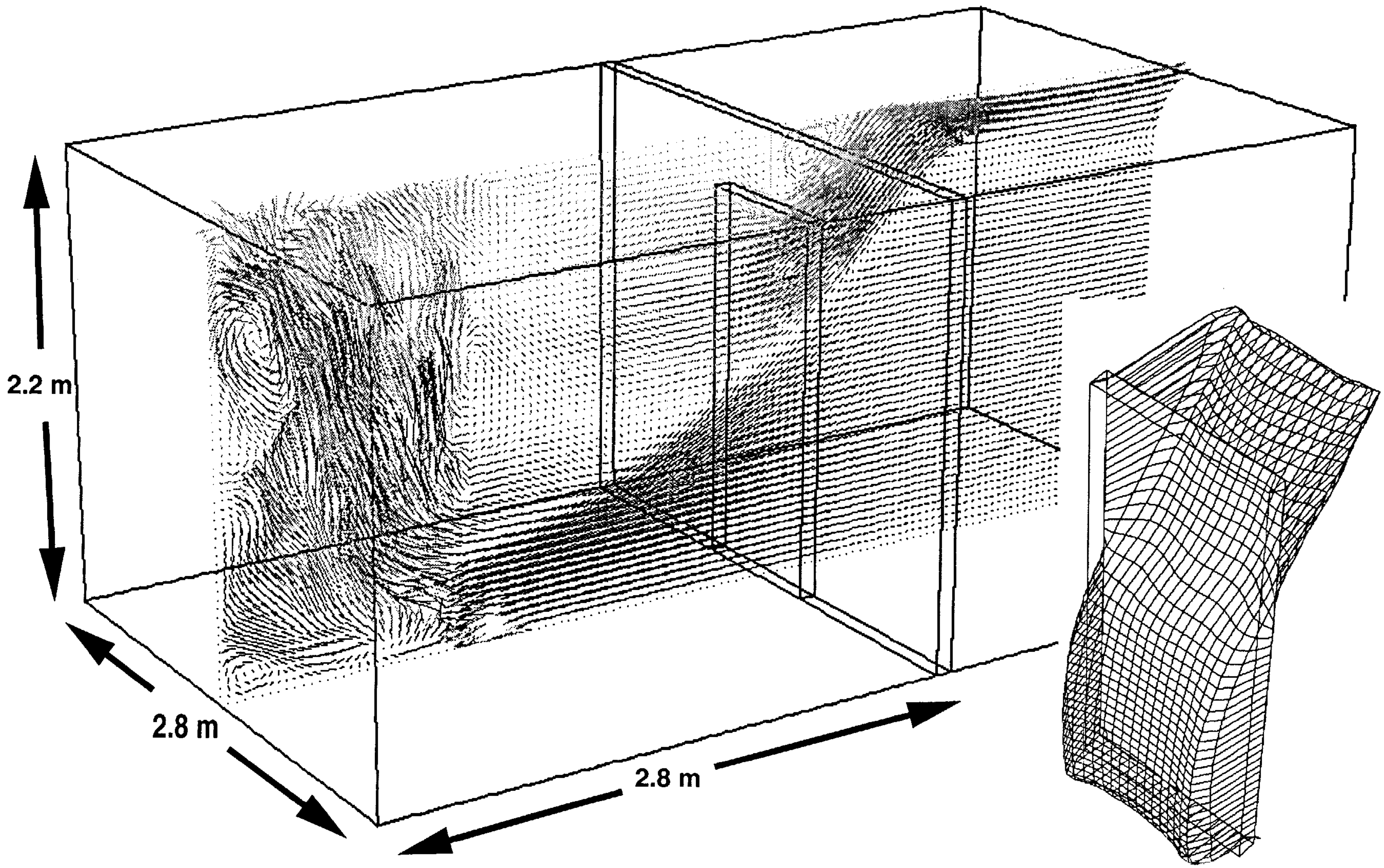
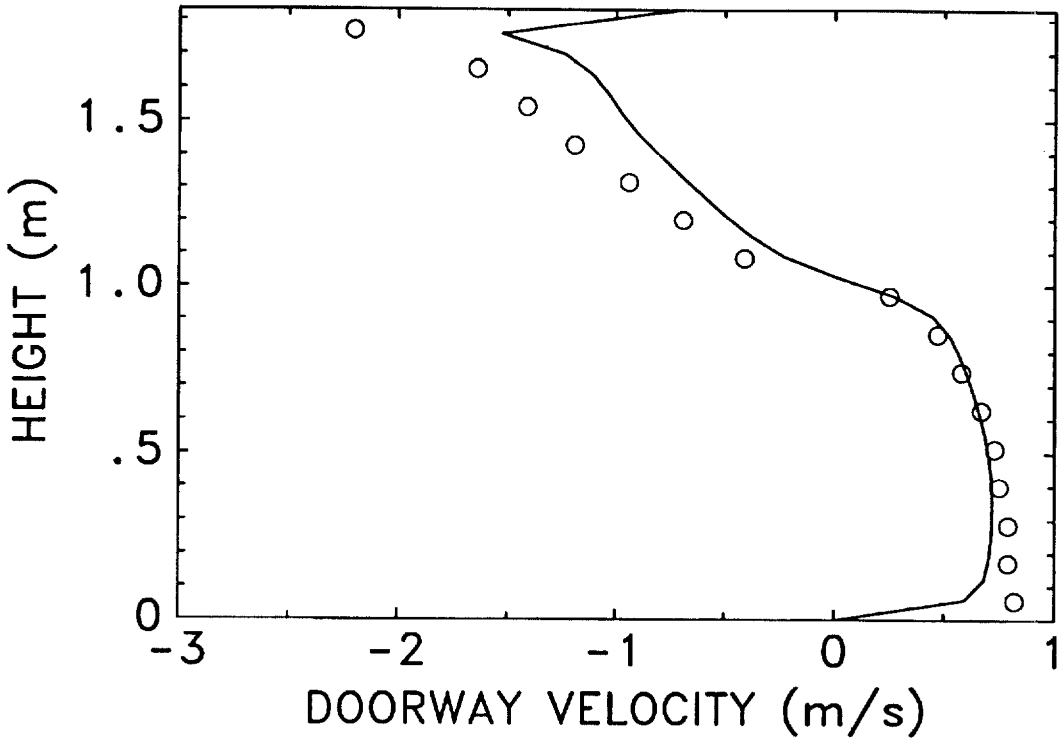


Figure 1. Velocity vectors in vertical center plane of the simulation of Steckler *et al.* experiments. Inset at right shows wire frame display of doorway velocity profiles. Note that velocity maximum at each height occurs at edge in agreement with Figure 5 of Reference [4].



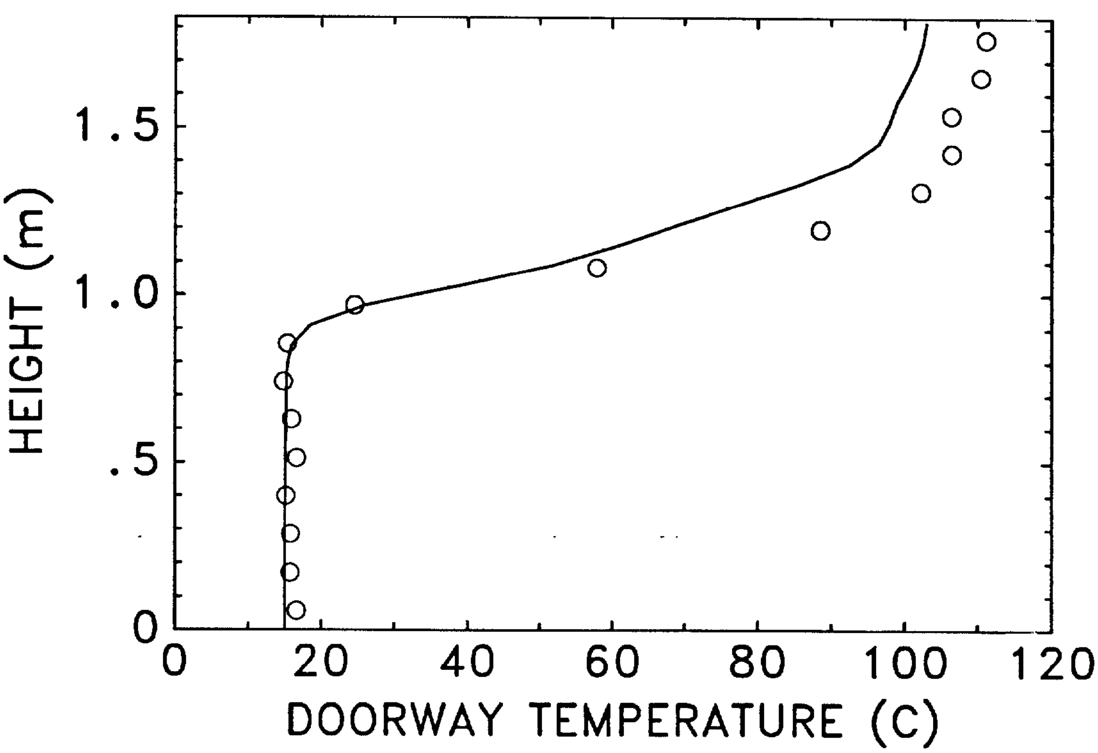


Figure 2. Velocity and temperature profiles in the center of the doorway in the Steckler *et al.* experiments. The circles represent experimental data and the solid lines represent results of the simulation performed at 3 centimeter resolution.

The above form of the conservation equations emphasize the importance of the divergence and vorticity fields, as well as the close relationship between the thermally expandable fluid equations [1] and the Boussinesq equations for which the authors have developed highly efficient solution procedures [2], [3]. These are applied directly to the equations presented here with minor modifications and no loss in performance. The only changes from earlier methodology are a return to a uniform rectangular grid with blocks of cells masked to simulate internal boundaries; and the use of a second order Runge-Kutta scheme to advance the velocity and temperature fields in time.

The fire is represented by introducing a large number of Lagrangian elements which release heat as they are convected about by the thermally induced motion. Since the fluid motion determines where the heat is actually released, and the heat release determines the motion, the large scale features of the coupling between the fire and the smoke transport are retained. It should be noted, however, that the heat release rate is *not* predicted, but is an input parameter in the computer programs implementing this model. The smoke is followed by continuing to track the convected elements after the fuel burnout is completed. A specified percentage of the fuel consumed is assumed to be converted to smoke particulate. Thus, a knowledge of the spatial distribution of the Lagrangian elements is equivalent to a specification of the smoke particulate density at any instant of time. The spray droplet drag density is determined by computing a large number of Lagrangian water droplet trajectories in a quiescent fluid. This technique permits the future substitution of a more realistic spray model and/or experimental spray data without changing the basic approach to smoke movement.

3 Results

Three examples illustrating the present capabilities of the approach outlined are presented. The first, a simulation of enclosure fire experiments conducted by Steckler et. al. [4], [5], shows that reasonably good agreement with experimental results can be obtained at the levels of spatial resolution achievable with current CFD techniques and computer facilities. The second, a study of smoke movement induced by a fire in a hypothetical hotel unit, demonstrates the level of geometrical complexity that can be simulated at present. These simulations are performed at 3 and 4 cm. spatial resolution respectively. The third example is a ceiling jet advancing down a long corridor. It is inspired by a series of experiments performed by Prof. Zukoski.

The overall geometry of the Steckler et. al. experiments is shown in Figure 1. The velocity vectors displayed in the vertical center plane after the flow has reached an apparent steady state are also shown. In addition to giving some idea of the overall flow pattern they give an indication of the spatial resolution achieved in the computation. The wireframe doorway velocity plot shows the characteristic orifice profile, with the maximum speed near the jet edge. This plot is remarkably similar to that given in Figure 5 of Reference [4], where the experimental profiles are displayed. A quantitative comparison between theory and experiment is shown in Figure 2, where time averaged doorway centerline velocity and temperature profiles are displayed. There are no adjustable parameters in the model, so the relatively good agreement between the measured and calculated results is a reasonable indicator of the *predictive* capability of the present approach.

A simulation of a fire on top of a bed in an idealized hotel room unit is shown in Figure 3. The unit also contains a sofa to the right of the bed, as well as a chest of drawers and a desk on the opposite wall. A closet blocked off from the rest of the unit and a bathroom with open doorway are to the left. Air heated $10°C$ above ambient enters the room at 25 cm./sec. through a duct on

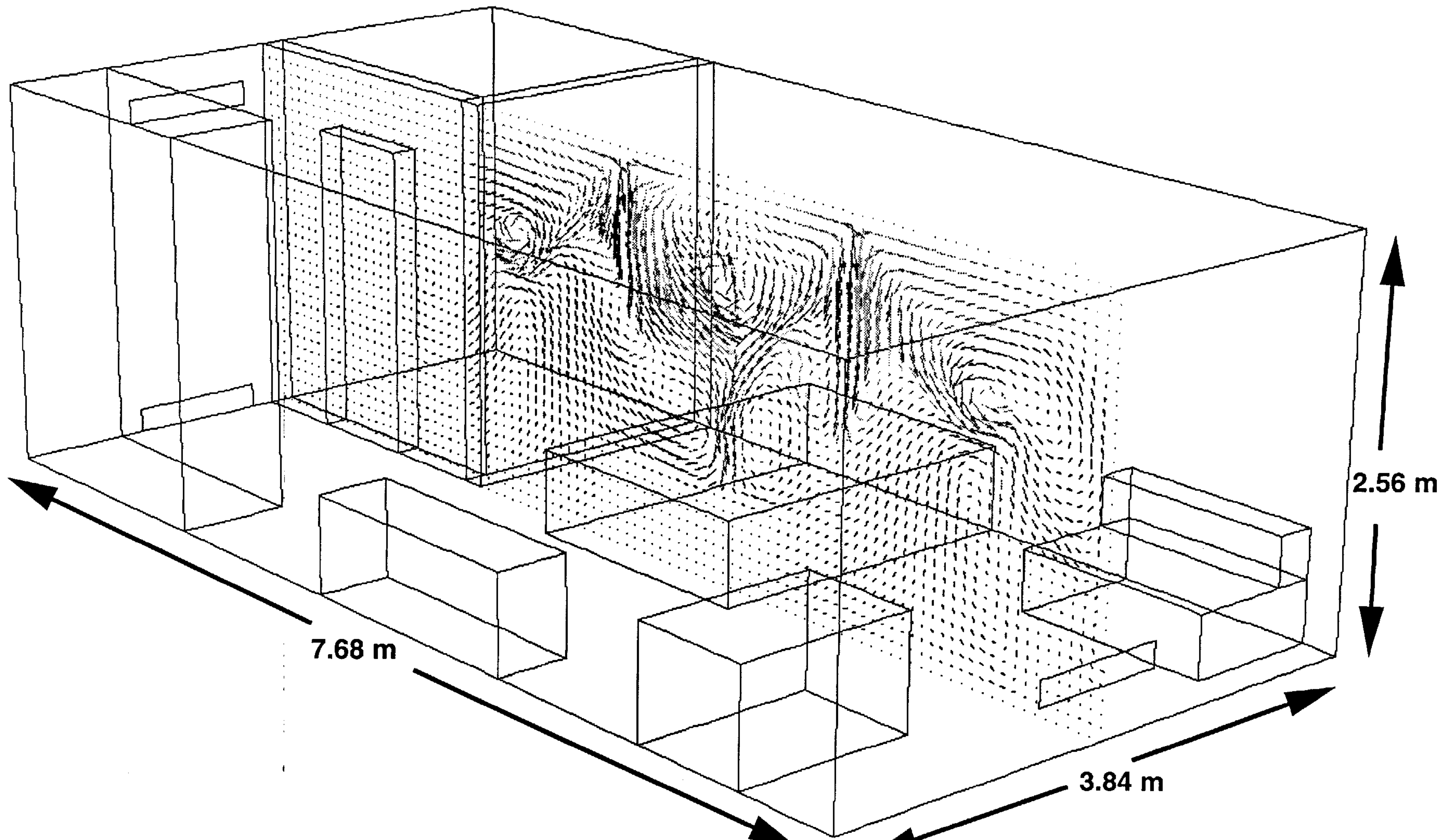


Figure 3. Velocity vectors in the vertical center plane of room 20 seconds after fire initiation. Two sprinklers sited immediately above the bed have just begun to inject water spray at 2 liters/second each. Every other vector in each coordinate direction is shown for clarity. The overall grid size is 192x96x64 cells corresponding to 4 centimeter spatial resolution.

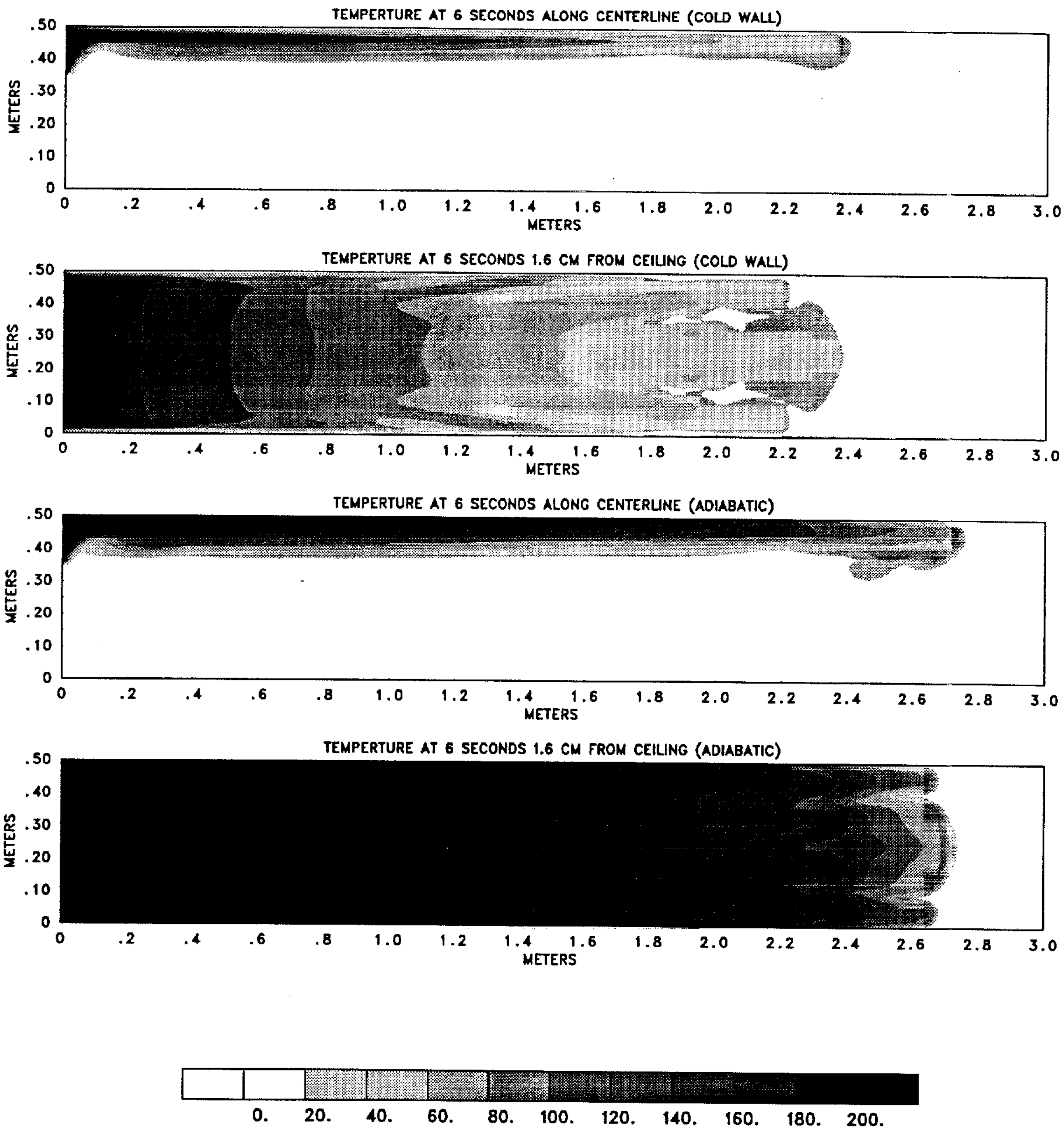


Figure 4. A comparison of two gravity currents, one run under cold wall conditions (top 2 figures) and one run under adiabatic conditions (bottom 2 figures). The grid size for each run was 324x54x64 cells, with the size of the grid cells varying in the vertical direction so that the cells near the top of the enclosure were about half a centimeter thick. The temperature of the gas exiting the vent is 212 C. The shades of the contours represent temperatures in excess of ambient (15 C).

the lower right wall and is extracted on the upper left wall above a closed door with a 2 cm. gap at the floor. The vents operate at fixed outside pressures, so the inflow is reduced and outflow increased as the room pressure rises due to the fire. Figure 3 shows the velocity vectors in the vertical center plane down the length of the room 20 seconds after the fire begins. Only 1/4 of the vectors are shown in the interests of clarity. The overall grid is composed of 64x96x192 4 cm. cubes. Two sprinklers located on the ceiling near on either side of the bed have been triggered. The force fields generated by the sprays are calculated in advance and activated either at a prescribed local ceiling gas temperature or a set time. The calculation simulates about one minute of real time. These computations required approximately 20 microseconds per cell per time step on an IBM RS 6000/58H server, and used 280 MBytes of memory.

Figure 4 shows temperature contours from two simulations of gravity currents generated by injecting air heated to 212°C at 25 cm/s into a 6x1x1 0.5 meter high corridor containing stagnant air at 15°C. The upper plots show top and side views with the walls held at 15°C while the lower two correspond to adiabatic boundary conditions. The cold wall boundary conditions generate intense axial vortices which greatly enhance the ceiling heat transfer and rapidly reduce the temperature in the ceiling jet. Since the force driving the gravity current is the buoyancy induced by the temperature rise, this leads to a rapid slowing of the ceiling jet. These 'convection rolls' were noted explicitly in [6]. The computations were performed using a 324x64x54 grid with a variable grid in the vertical direction.

These examples are intended to demonstrate that smoke movement caused by enclosure fires can be calculated with reasonable accuracy directly from the underlying Navier Stokes equations in scenarios of practical interest. While many other physical mechanisms need to be included before a full predictive capability is achieved, it is clear to us that the methodology outlined above is the only currently available way of *guaranteeing* increasingly accurate predictions of smoke movement in the future.

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Discussion

Patrick Pagni: I just wanted to start with a comment before the question that it's really appropriate to have the best of modern computational fluid mechanics presented at a symposium honoring Ed Zukoski. Howard, looking to the future, could we have your vision on the right way to add radiation to this problem to the same level of accuracy that you have the fluid mechanics modeled?

Howard Baum: I'd like to answer in two parts. First, I'd like to say something about your first comment. The thing which actually has sustained us over the last few years and gotten us to plunge this far into it after wandering in the desert for a while is Ed Zukoski's salt water experiments. And, in fact, if it wasn't for the both the beautiful simplicity and clarity of those experiments, simple enough so that even I could understand them, then we would not have been able to get some kind of experimental confirmation that this work was on the right track three or four years ago. As to the radiation calculations, we are embarking on them now and the thing which I will say is the crucial part is to not to try to believe that we can predict the radiation from the temperature fields that we calculate. Just as we have these elements moving with the fluid that is releasing chemical energy, we can say that some fraction of that chemical energy is emitted as thermal radiation into the bulk of the gas. And we are then arguing that subsequently, it is either absorbed or not, depending upon the amount of smoke in the gas in the room or in the outdoor plume or whatever. We are just beginning these calculations now and are still developing methodology. So at this point, the only thing that I can say is that this is the approach that we are following and I hope in several months to have something tangible to show for it.

Ronald Alpert: Do you think the trend is going to be in the near future for soaking up the added computational capacity of new machines as they get faster and faster? Is the trend going to be to add more and more physics to the problem, such as thermal radiation, such as putting in the complete two way interaction between sprinkler water droplets and the flow and other such things? Or will the trend be to get better resolution as you have implied?

Howard Baum: For the immediate future for us, I see basically two aspects to the research; one is to hold the spatial resolution fixed and consider more complicated geometries just for smoke movement. I've shown you simulations for a motel room or what you might think of as a bedroom. We believe that the computing capacity exists right now to do that for the equivalent of an office suite or a small house. The second leg of this, which we have already embarked on, is to assume, whether rightly or wrongly, that we have gone far enough with the spacial resolution that we currently have and try to add radiation, which we are actively doing. And we have some simple trajectory models for a sprinkler spray that has to be modified, for example, to make it obey Newton's laws of motion and to gradually increase the amount of physics in the calculation. One last thing as part of that, we want to, rather than postulate what happens on these little small scaled elements moving through the fluid, we want to actually study them as a combustion problem in their own right. Dr. Ruddy Mell, who is working with me as an NRC post-doc, is, in fact, embarked on an investigation of that problem.

Discussion cont.

Richard Gann: Having heard the answers to the last two questions, I feel compelled to put in a bid for one more facet. I'd like to get your views on the capability of adding the spacial and temporal extensiveness of the heat release and chemical species changes as opposed to making them essentially a source term and instantaneous.

Howard Baum: The problem that you are addressing is basically as complicated an issue as everything that I have talked about here. But I think it is important to say what the origin of the complication is. That is, if the chairs that we are all sitting on catch fire, we do not have a clue as to what those fuels really are. If that whole problem of condensed fuel degradation could be understood at a level that would yield predictions on a species-by-species level, then I think the ability probably exists. Not in my head and not in our collaborators. But there are other people in the combustion community who will calculate fairly elaborate chemistry, at least in laminar flames and simple situations. So if that problem could be solved, I could imagine a future, not next year, but at some point when these little elements were actually carrying along real chemical composition calculations and drawing on the local environment that they were seeing to provide the oxidizer visited or not. But my colleague Takashi Kashiwagi informs me that you could write a book just on the reactions that go on in paper and therefore, I believe that some rationalization of the way in which we approach the burning of solid materials is really required before one can even contemplate the next step in gas phase combustion.