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Prediction of Smoke Movement: An Overview of Field Models

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ABSTRACT

This paper reviews the mathematical and physical basis of field models used for fire and smoke movement prediction and their application to a number of experimental situations for which validation data are available. The models involve the numerical solution of basic equations governing three-dimensional, steady, and transient flows with prescribed boundary conditions. The effect of turbulence, combustion, and radiation are included with various models.

The models predict the flow behavior quite well. Temperature and velocity distributions show very good agreement with data; gas concentrations are less well predicted. The generality of field models permits their use in large-scale situations where simple models might be inapplicable.

INTRODUCTION

The successful development of numerical techniques to solve the basic equations of fluid mechanics has led to their extensive use for design and analysis. The use of mathematical models based on these techniques to predict the behavior of fire and smoke movement has been no exception, and a number of applications have been reported in the last few years. The essential feature of numerical methods is very simple. The flow domain is divided into numerous small volumes. Equations representing the conservation of momentum, energy, species concentration, etc., are solved at a point within each volume. This procedure results in large systems of equations, which, because of their nonlinearity, require iterative solution and, ideally, large computers to solve them rapidly.

The great advantage of this approach is that information is obtained at every computed point in the flow domain. A more complete picture of the flow situation is built up, and this fine detail permits the use of more mechanistic representations of the processes that are occurring. For example, local heat release due to chemical reaction can be related to species concentrations, reaction kinetics, and temperature within a cell. Mathematical models of this kind therefore remove some of the need for empirical approximations used in simpler models and hence preserve a greater generality. The ability to alter the assumptions on which the physical processes are based and to test them with a mathematical model is also useful, and encourages a closer scrutiny of the relevant physics. Such models might well provide a framework for investigating processes such as flashover and flamespreading.

This paper attempts to review the status of the socalled "field" models with which the author is most familiar in terms of their mathematical basis, applications, and present level of validation. Field models are based on the solution of the fundamental equations governing all fluidflow situations. They employ mathematical techniques that have been and continue to be developed in areas such as aerospace and nuclear energy. They are therefore well founded, and benefit from advances being made in these areas, e.g., the use of distorted grids to enable easier geometry definition and improvements in the ease of use of computational fluid-dynamics methods in general.

Inaccuracies in a mathematical model can arise from two sources—either numerical or physical. Numerical errors can occur, for example, when the grid size is too coarse, and gradients within the flow are not properly resolved. The cure is simply to refine the grid, but by how much? Since the answer is not known in advance it has become common practice to set up a problem using a relatively coarse grid, and then refine the grid progressively until no significant change in the predicted values is observed.

Applications of field models have been performed by fire researchers and architects. The former have provided most validation material. Cases where model prediction and experiment have been compared include room and compartment fires, tunnel fires, and a simulated six-bed hospital ward, a one-sixth-scale sports hall, and an airplane. Architectural applications have been aimed at predicting smoke behavior for buildings under design, particularly large structures where the empirical content of zonal models may not be applicable. In such circumstances field models have been used as design tools to assess the fire risks associated with the design. It is encouraging to observe that sufficient confidence has been built up in the use of field models that they can be used for such a purpose.

The next section of the paper provides an overview of the mathematical basis of field models, and briefly describes some of the physical model enhancements that have been implemented in some models. Application studies are described in the following section, and the predictions are compared with data.

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MATHEMATICAL ASPECTS OF FIRE AND SMOKE MODELING

The equations that need to be solved for any fluiddynamic problem can be written in the following general form:

$$\frac{\partial}{\partial t}(r\varrho\varphi) + \operatorname{div}\left(r\varrho v_{\varphi} - r\Gamma_{\varphi} grad_{\varphi}\right) = rS_{\varphi}$$

where

r = phase volume fraction; $\rho =$ density

 φ = dependent variable, v = velocity vector Γ_{φ} = exchange coefficient (laminar or turbulent); and S_{φ} = source or sink terms.

The computer solves a form of the above equation, which is obtained by integrating over a control volume. The solution methods are well established, reliable, and widely used. Further details can be found in Spalding (1981) and Gosman et al. (1969).

TABLE 1 Exchange Coefficient ($\Gamma_{\!\varphi})$ and Source Terms (${\rm S}_{\!\varphi})$ for Different Variables

φ	Г,,,	Sø
1	o	0 (Continuity)
u	^µ eff	$-\frac{\partial p}{\partial x} + \frac{\partial}{\partial x} (\mu_{\text{eff}} \frac{\partial u}{\partial x}) + \frac{\partial}{\partial y} (\mu_{\text{eff}} \frac{\partial v}{\partial x})$
		$+ \frac{\partial}{\partial z} (\mu_{\text{eff}} \frac{\partial w}{\partial x})$
v	₽eff	$-\frac{\partial p}{\partial y} + \frac{\partial}{\partial x} (\mu_{eff} \frac{\partial u}{\partial y}) + \frac{\partial}{\partial y} (\mu_{eff} \frac{\partial v}{\partial y})$
		+ $\frac{\partial}{\partial z}$ ($\mu_{eff} \frac{\partial w}{\partial y}$)
w	µeff .	$-\frac{\partial p}{\partial z} - g (\rho - \rho_{ref}) + \frac{\partial}{\partial x} (\mu_{eff} \frac{\partial u}{\partial z})$
		$+ \frac{\partial}{\partial y} (\mu_{\text{eff}} \frac{\partial v}{\partial z}) + \frac{\partial}{\partial z} (\mu_{\text{eff}} \frac{\partial w}{\partial z})$
h	$\frac{\mu_{\rm eff}}{\sigma_{\rm h}}$	ġ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,
k	$\frac{\mu_{eff}}{\sigma_k}$	$G_k - \rho \epsilon + G_b$
ŧ	$\frac{\mu_{eff}}{\sigma_{\epsilon}}$	$\frac{\epsilon}{k} [(G_k + G_b) C_1 - C_2 \rho \epsilon]$
μe	ff = µt +	$\mu_{\ell} \qquad \mu_{t} = c_{\mu} \rho k^{2}/\epsilon$
_{Gk}	- µt {2 [$(\frac{\partial u^2}{\partial x}) + (\frac{\partial v^2}{\partial y}) + (\frac{\partial w^2}{\partial z}) + [(\frac{\partial u^2}{\partial z}) + (\frac{\partial w^2}{\partial x})]$
	+ $\left[\left(\frac{\partial w^2}{\partial w}\right)\right]$	+ $\left(\frac{\partial v}{\partial z}\right)^2$ + [$\left(\frac{\partial u}{\partial z}\right)^2$ + $\left(\frac{\partial v}{\partial z}\right)^2$] , and

The buoyancy production term, G_b, represents the generation/suppression of turbulence due to buoyancy. In stable stratification (fire enclosures), ag/az is negative; hence Gb becomes a sink term, and the turbulent mixing is reduced. The turbulence model contains six empirical constants that are assigned the following standard values: $C_1 = 1.44$, C_2 = 1.92, C_{μ} = 0.09, σ_k = 1.0, σ_{ε} = 1.3, and σ_h = 0.85.

The dependent variable, φ , can represent the fluid velocities in each coordinate direction for single- or multiphase flows, enthalpies, species concentrations, turbulence quantities, radiation fluxes, and so on. The number of differential equations that can be used to represent a problem need not be limited when such a computational approach is adopted. The limitation is more likely to be in the degree of understanding of the relevent physics, whether suitable exchange coefficients and source terms can be formulated. Table 1 gives some examples of the values of Γ_{ω} and S_{ω} for equations commonly solved in field models.

The flow behavior during a fire is usually threedimensional and is strongly influenced by turbulence and buoyancy effects. The simplest field models, therefore, need to solve equations for velocity in the three coordinate directions (u, v, and w), enthalpy (h), and pressure (p), and would employ a fixed value of turbulent viscosity (μ_i) to represent the effects of turbulent mixing and a prescribed heat source to represent the fire. The limitations that are applied by assuming fixed values of these quantities can be relaxed by solving additional equations and representing the various phenomena on a cell-wise basis rather than a global one. Such refinements to this basic model might include:

 The use of a turbulence model. The two-equation model in which the kinetic energy of turbulence (k)and its rate of dissipation (ϵ) are solved has been used in many of the studies reported here (see Table 2). The turbulent viscosity in each cell is then calculated from:

$$\mu_l = c \mu \varrho k \frac{2}{s}$$

where °µ is one of the turbulence model constants (see Table 1).

- A combustion model, which requires the introduction of additional equations to predict the concentrations of reacting and inert species, and source terms involving details of any kinetically controlled reaction rates. The simplest combustion model assumes a diffusion-controlled, single-step reaction, which may be represented simply as fuel + oxidant → product. This implies that any fuel within a cell will react instantaneously with any available oxidant. A mixture fraction equation (f) is required in this case. If chemical kinetic influences are to be included, then a further transport equation for the mass fraction of fuel (m_{fu}) is required, and a prescription of the reaction rate. The most common formulation for the reaction rate is to take the minimum of the laminar Arrhenius expression or that deduced from eddy break-up concepts proposed by Spalding (1971, 1976).
- A radiation model, in which ordinary differential equations are solved for the radiant fluxes. This introduces further physical questions regarding the absorption and scattering coefficients of the medium and emmissivities of the surfaces. Radiation models of this kind do not appear to have been used extensively, it being more common to use an enhanced wall heat-transfer coefficient to estimate

 $G_{b} = \frac{\mu_{t}}{\rho} g \frac{\partial \rho}{\partial z}$

TABLE 2 Summary of Experimental Cases and Mathematical Model Details

EXPERIMENT	DIMENSIONS (Length x Width x Weight)	NATURE OF HEAT (kW) FIRE SOURCE RELEASE
Swedish National Testing Institute: Test Compartment	in meters 3.6 x 2.4 x 0.8 0.8 x 2.0 door opening	Propane Gas 250 burner, rear wall
NBS room fire experiments	2.8 x 2.8 x 2.18 0.74 x 1.83 door 0.99 x 1.83 openings	Gas Burner 31.6,62.9 Center of Room 105.3,158.0 0.9 m ²
LINL TEST Cell	6 x 4 x 4.5 <u>Outlet</u> 0.65m square duct 3.6m above floor <u>Inlet</u> 2 x 0.12 slit; 0.1m move floor	Isopropyl 400 alcohol: (400 l/s 0.91m diam. air Steel pan; extraction) natural pool fire
ZWENBERG Tunnel	390 x 5 x 4 Pe One end closed,	trol Fire 14450 (2001) Nat.cover in 2.6m square 20250-2m/s tray 24950-4m/s
NRC/SNL/UL	6.5 x 4.25 x 3.0 1.2 x 2.4 door or 2.4 x 2.4 in (expt.2).	Heptane pool 600-900 0.3 x 1.5 pool Time-varying on wall opposite doorway.
FRS HOSPITAL WARD	7.85 x 7.33 x 2.7	0.45 x 0.5 t = polyrurethane 0-3m 5 foam mattress 3-7 20 0.25m from wall, 7-12 80
SHIMIZU CONSTRUCT. CO.	34 X 28 X 11.6 Forced ventilation	Pool Fire ?
JSS-Aircraft	17.1 X 3.3 X 2.1	Fuel pan 239 0.61m X 0.61m t=0 - 6m (4.52 of fuel) 50.7 t=6 - 10m

MODEL INFORMATION 2-EQUATION RADIATION COMBUSTION MODEL Steady Kinetically controlled eddy break-up model Steady х Fixed heat varies source with height Kinetically Steady x 1 controlled eddy break-up model x х Steady Kinetically controlled eddy break-up model Transient Heat release as input Transient Kinetically Х controlled eddy break-up model Transient Kinetically X controlled eddy break-up model Kinetically controlled eddy break-up model Transient (1st 4 minutes) X

the heat losses by convection and radiation. Similar assumptions to those used in zone models are frequently applied. See, for example, Kumar and Cox (1985).

Finally, it is necessary to describe the details of the boundaries in the mathematical model. A no-slip boundary condition is applied on solid walls for velocity components. Fluxes of momentum and heat can be predicted from wall function relationships. (See, for example, Launder and Spalding [1972].) Heat losses through the walls can be calculated from the wall conductivity and the local temperature gradients that are predicted.

On free boundaries, it is conventional to impose a fixed reference pressure. The mass inflows and outflows to the domain are then an outcome of the calculation. To ensure the validity of this, such boundaries should be sufficiently remote that they exert no unphysical effect on the solution. In fire-modeling applications, the boundary is usually fixed a little distance away from doorways in order to avoid such problems.

FIELD MODEL APPLICATIONS

This section presents the results of studies in which mathematical models have been applied to predict particular experiments. The experimental cases include room fires investigated by the Swedish National Testing Institute (Sundstrom et al. 1981), the National Institute of Standards and Technology (formerly National Bureau of Standards) (Steckler et al. 1982), and a national laboratory (Alvarez 1984); a tunnel fire (Fiezlmayer 1976); a nuclear reactor scenario (Cline et al. 1983); a simulated hospital ward experiment carried out by the Fire Research Station (Kumar et al. 1985) a one-sixth-scale sports hall investigated by a construction company (Pericleous et al. 1988); and an airplane fire (Kumineca and Bricknav 1982). Table 2 summarizes the details of these experimental cases in terms of overall dimensions, the nature of the fire source and the heat release, whether steady or transient conditions are established, and some details of the modeling strategies. It should be noted that models reported in this paper are those jointly developed by the Fire Research Station and CHAM. The two-dimensional steady code MOSIE 2 was the first such development, followed by JASMINE, a threedimensional transient version. The current JASMINE program utilizes the general-purpose CFD code PHOENICS to solve the required equations.

Most of the experimental cases used a liquid or gaseous source of fuel for the fire. The main chemical reac-



Figure 1 Swedish test room: typical numerical prediction illustrating flow visualization

tions and the heat release therefore can be calculated with reasonable accuracy, if complete combustion is assumed.

The experimental measurements reported tend to be broadly similar for most of the experiments. Thus, the information usually available for validation comprises:

- The mass balances for the system in terms of inflows and outflows.
- Gas velocity and temperature distribution at doorways as functions of height.
- Point temperature measurements within a room.
- Thermocouple rakes that provide horizontal and vertical temperature distributions.
- Point gas concentration measurements, e.g., CO₂ and O₂.

The field model can readily provide information to compare with these data, as well as giving both a broader understanding of the overall flow behavior and detailed structure where required. Figure 1 shows, for the Swedish test room case, typical computer-generated plots obtained from a field model. Figure 1a shows a velocity vector plot at the room symmetry plane. Each vector corresponds to a grid-point location and represents the magnitude and direction of the gas velocity in that plane. Temperature contours are shown in Figure 1b. These illustrate the noticeable stratification of temperature and the rapid rise above the fire source. A three-dimensional representation of the flow is

Figure 3 NBS case: doorway velocity and temperature profiles

possible by plotting particle tracks, as in Figure 1c. These show the entrainment of air through the door, its rise in the region of the fire, some flow recirculation, and finally its exit at the top of the door.

Temperature and Velocity Prediction

The comparison of model results with experiment for the Swedish test room (Markatos and Pericleous 1983) is shown in Figure 2. The doorway velocity profiles at the symmetry plane are shown in Figure 2a, and the temperature profile in Figure 2b. The velocity is negative in the lower half, indicating entrainment into the room, and positive outflow occurs at heights above 1.0 m. The agreement with experiment is reasonable except at the ceiling, where the velocity is underpredicted by about 20%. The shape of the temperature variation at the door is well predicted, although some displacement from the experimental value can be observed.

Figure 3 shows doorway velocity and center temperature profiles for the NBS room fire and the JASMINE model (Cox 1983; Cox and Markatos 1984). Here again, the agreement is good, although with some discrepancy occurring between the hot and cold layers. The relatively coarse computational grid (13 by 12 by 12) may have had some small influence (Cox and Markatos , 1984). This may indicate weaknesses in the mathematical model in the area of turbulent mixing prediction.

The Swedish and NBS test cases are for naturally ventilated rooms. In contrast, the national laboratory experiment employed forced ventilation, extracting 400 to 500 L/s of air from the room, and allowing inflow through a slit at floor level. Vertical thermocouple rakes have been used to measure the variation of temperature within the room, 1.5 m on either side of the fire tray, and on one of the walls and the ceiling. The JASMINE predictions, reported in Cox and Kumar (1984), are compared with the experiment in Figure 4. Here again, comparison is quite good, the model predictions giving a reasonable average of the experimental data. Larger errors occur at the floor and ceiling, and it is reported in Cox and Kumar (1984) that this may be due to simplified wall heat-transfer assumptions, the coefficient having been fixed to 20 W/m²K.

Figure 5 shows JASMINE temperature predictions and experimental data for the tunnel fire prediction reported in Kumar and Cox (1985). The comparison with data is not as good as the room fire tests described above,

Figure 4a LLNL test case: case temperature vs. height

Figure 4b LLNL test case: wall and ceiling temperature vs. height

particularly in the region above the fire source. Errors are particularly significant in the natural convection case. The use of a fixed turbulence viscosity and a simplified combustion model may have been the cause of the poor agreement for this case. Difficulty in converging the solution for the natural convection situation necessitated these simplifications. The forced convection cases show much better agreement probably because they employ more detailed models.

Prediction of the transient fire situations, caused by variable heat releases, which were investigated by the NRC, FRS, and SCC, are reported in Kumar et al. (1985), Pericleous et al. (1988), and Boccio et al. (1985). Point temperature measurements as functions of time are given for the NRC experiment in Figure 6. These show data at 1 ft, 2 ft, and 3 ft below the ceiling and 3 ft above the floor. The rise and fall in temperature with time follows the variation in heat release during the experiment. It is interesting to note that the heat release was a combination of a heptane pool fire and burning cables. The predictions agree quite well with the experimental values except at the peak

1

Figure 5 Tunnel fire: temperature measurements compared with prediction for natural and fired ventilation cases

temperature; the maximum temperatures being underpredicted by about 15%. The predicted rise in temperature is not as sharp as that observed in the experiment, and this applies to the other simulated cases described in Boccio et al. (1985). The longer computation times associated with three-dimensional transient calculations may have necessitated a coarser grid (950 cells in this case) than is desirable for numerical accuracy.

The hospital ward (Kumar et al. 1985) and the sports hall (Pericleous et al. 1988) both had an initial flow distribution, the former caused by convection heaters on one wall and the latter by forced air fans. The initial conditions for these predictions were therefore obtained by performing a steady-state calculation prior to running the transient. Figures 7 and 8 show temperature data from these tests.

Figure 7 FRS hospital ward fire

The hospital ward results, Figure 7, show the variation above the fire and at several locations in the room. All the results show reasonable agreement. Figure 8 shows similar results for the sports hall.

Predictions for the airplane fire (Kuminecz and Bricknev 1982) are reported in Galea and Markatos (1987). As with the sports hall, a distorted grid was used to facilitate representation of the air plane geometry. Figure 9 illustrates the temperature variation along the airplane at one and four minutes after the fire has started. The general shape is correctly predicted, but the value is everywhere higher than the experiment. Grid studies carried out for a quasisteady simulation indicated a strong effect, and that quantitatively accurate results could not be expected for the grid used in the transient calculation. It is interesting to note that the grid studies indicated a lowering of the temperature at the centreline grids. It might be expected, therefore, that better agreement could be obtained for the transient case if a finer grid were used.

Taking the above results as a whole, and bearing in mind that each case is unique in its geometrical features, location, and strength of fire source, it can be concluded that the field models have been quite successful at predicting temperature within the test rooms and the conditions at exit. The major features of the flow structure must therefore be quite well predicted for this to be the case. There have been rather few grid studies performed, and most of those reported indicate only a small effect of grid size on temperature predictions. The noticeable exception is the airplane fire, which did show a stronger dependence.

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Figure 9 Airplane fire: temperature variations along the cabin

Species Concentration Prediction

There are fewer measurements of gas concentrations in the literature. Time-varying CO_2 measurements are available for the hospital ward fire, and CO_2 and O_2 measurements for the tunnel fire and national laboratory room fire. Figure 10 shows the hospital fire case CO_2 variation at two locations with time, and the vertical variation after 12 minutes. It seems that the concentration is reasonably well predicted at "nose" height, but is poorly predicted at "bed" height. The vertical variation illustrates the overprediction further, particularly at the lower levels.

The tunnel fire predictions are compared in Table 3. They agree fairly well in most cases. However, the size of the experiment and the sparseness of measurements do not make it a particularly good case for validation purposes, and it is almost certainly the case that a fine computational grid would be required before quantitative comparisons could be made.

Figure 10a FRS hospital ward fire: CO₂ concentration—time variations at two heights

In the national laboratory test case, the measured exit concentrations of O_2 and CO_2 were 10.4% and 7.5%, respectively. The corresponding predicted values were 14% and 5.5%. This appears to be a similar level of accuracy to the other cases.

Mass Inflows and Outflows

Data are available for integrated mass inflows and outflows for three of the cases—the Swedish test room and the NBS and national laboratory experiments. Comparisons are made in Table 4 with predicted quantities. It can be seen that they compare well. The worst error is about 17% for the Swedish test cases; the other predictions are within 10% or less.

CONCLUDING REMARKS

This paper has provided a general outline of the mathematical and physical basis of field models that have

Figure 10b FRS hospital ward fire: CO₂ concentration—height variation 12 minutes after ignition

TABLE 3 Predicted (P) and Measured (M) Values of O₂ and CO₂ Concentrations

a) Natural Ventilation

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b) Forced Ventilation of 2m/s.

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c) Forced Ventilation of 4m/s

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		1		1		۱	0.5	• •		1	0.9	1	0.8	1	1.9	1 3	2.3	1		1		1		1	

been used for the prediction of fire and smoke movements. These models are based on the numerical solution of the basic equations of fluid motion and therefore represent a fundamental approach to the problem of prediction. They require assumptions to be made by the user for the characterization of effects such as turbulence and combustion, and various models exist for incorporating into the framework of a field model.

The validation studies that have been performed indicate that the major flow characteristics resulting from the fire source and ventilation arrangements can be predicted by the models. Quantitative comparison is good for temperature and, where available, velocity data, but not as

TABLE 4 Experimental and Predicted Total, Mass Flow (kg/s)

	MEAS	CTED	REMARKS		
	IN	OUT	IN	OUT	
Swedish Test Room	1.01	0.89	.84kg/s	.84	
NBS	0.446 .56/.605 .624 .688 .677		.475 .555 .617 .657 .683	.476 .557 .622 .665 .684	31.6 kW 62.9 kW 105. kW 158. kW 629. kW
LINL	0.3	0.24	.269	0.257	

good for gas concentrations. Virtually all of the studies reported have used quite coarse computational grids. Grid studies have shown little dependence of temperature variations on nodalization, with one exception. Gas concentration measurements have not been subject to the same examination. Therefore, no clear guidelines exist for the user of field models in terms of nodalization, and it may be the case that the choice of grid is dependent upon the geometry to such an extent that each case should be examined individually for numerical accuracy.

Long computer times, on the order of several hours, are an obvious disadvantage of field models. While this should not be a consideration where fire safety is concerned, it is nevertheless a factor in the choice of design approach. Before embarking on a field-modeling exercise, the user must be certain that the results will justify the additional complexities of the approach. The architectural application mentioned earlier was one in which zone models were not deemed to be suitable for the larger scale of building and, in order to obtain building permits, alternative justification of safety aspects was required. Given the level of validation described in this paper, the use of a field model does seem justifiable.

With the ever-increasing power of computers, it may soon become normal practice to use a field model for smoke-movement prediction and ventilation design. A more user-friendly model would be required and many safeguards would have to be incorporated before use of such a program by non-experts in computational techniques could be envisaged. An alternative role for the field model might be the development of design guidelines by numerical experiments rather than physical ones—the cost would certainly be less. The development of zone models might proceed in a similar way.

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