

# Computational Field Models in Fire Research and Engineering

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## ABSTRACT

Field models solve modelled conservation equations for mass, momentum, species and enthalpy in time-dependent turbulent flow driven by buoyancy. Detailed consideration is given to the submodels for the effects of buoyancy on turbulent transport and convective heat transfer, and for the combustion model on mean density and radiant emissivity. Improvements to existing state-of-the-art codes are suggested. Improving the credibility of field models requires a well-documented pedigree of validation of all submodels. Field models can give much needed qualitative and semi-quantitative information to both fire scientists and fire safety engineers. They can be expected to surpass zone models in use by the fire safety engineering profession in about five years.

**KEYWORDS:** Fire, field models, buoyancy, convective heat transfer, chemistry.

## INTRODUCTION

The computational field models of interest here solve the transient, three-dimensional Navier-Stokes equations and related equations for species and energy conservation in fires using turbulence models for turbulent transport. Laminar flames are also of interest in some fire science problems, such as fire spread. The code JASMINE [1-5], from the UK Fire Research Station, is a well known example of such a field model. The term "field" model is used to distinguish such models from zone models, such as the Harvard Fire Code [6], which make a priori assumptions about the structure of the flow field and divide it into zones in which the properties are assumed to be uniform. Friedman [7] reviews computer models for fire and smoke. Field models for fires belong to the generic and rapidly expanding subject of computational fluid dynamics (CFD) widely used in industrial aerodynamics and combustor design. Many commercially available CFD codes claim to have a fire modelling capability.

CFD is now well established as an important design tool in the engineering of many systems, including pumps, turbines, ductwork, air-conditioning systems, environmental flow, and combustors for furnaces and gas turbines [8-12]. Insights gained from CFD modelling greatly reduce development time during rig testing or commissioning. It is recognized that the results predicted are not fully quantitative but nevertheless they can be used with great benefit. Acceptance by the fire research and fire engineering communities has been much slower. Skepticism arises from the belief by some, e.g. [13], that fire plumes are dominated by large eddy structures and are not amenable to modelling based on any statistical approach. But it also arises from those with wide experience in turbulent flow modelling who understand the difficulties in modelling the complex buoyant flow involved and who are dismayed by those who glibly claim success with transparently simplistic models. The newly emerging profession of fire safety engineers are reluctant to adopt a modelling approach which lacks credibility and may be difficult to sustain in the courts. The legal framework in which they work is different to that of designers of most other engineering systems. Fire safety designs cannot be proven and fine-tuned with full-scale testing or on-site commissioning. Emmons [14] has predicted that simple models, such as zone models, will remain the workhorse of the profession with the more sophisticated field models remaining as a research tool.

For those committed, as I am, to the development of CFD as an engineering tool, these negative attitudes are disappointing, and will have to be overcome by improving our standards and putting our house in order. Field models are obviously much more powerful than zone models. Properly based and validated, and correctly used, they can give valuable insights and semi-quantitative answers into problems which are complex and for which there is no prior fire experience - and hence no basis for a zone model approach. Such problems include atriums, enclosed stadia, road tunnels, escalators in railway stations, aircraft, airports, and a host of industrial environments such as oil-rig platforms and coal-mine roadways. With the increased power of work-station computers now bringing field model calculations into the scope of everyday engineering budgets it seems that this is much the best way to go. Field models can also give valuable insights into traditional well-researched areas, such as fires in rooms and corridors. They could also greatly advance our understanding of the complex processes involved in fire spread and in the apparatus used for the testing of materials.

As an engineering scientist I recognize that there are many scientific deficiencies in the current state-of-the art. These deficiencies are not such as to require abandonment of the whole approach: research is needed to overcome these deficiencies by improving the relevant submodels for turbulent transport, radiation transfer, etc. I also recognize that, in the wrong hands, field models can give disastrously incorrect results. As an engineer I am concerned about the management of this human side of the problem. In fire engineering these scientific and human problems are particularly acute as the profession is striving to shake off a past of over-prescriptive codes and standards based on imperfectly understood "experience" to a future based on engineering science and the use of performance standards assessed in risk management terms [15, 16].

The aim of this paper is to consider in some detail a few of the important physical and chemical aspects of fire and the way in which they are incorporated into field models. I have limited my scope to those few areas where I have some expertise: buoyant convection, convective heat transfer and combustion modelling. JASMINE [1-5] is taken

as representative of the state-of-the-art. A general discussion follows concerned with the use of field models in fire science and engineering, the validation of the submodels used and general techniques for improving quality control.

## BUOYANT CONVECTION

We follow the presentation of Cox and Kumar [2]. The equations solved are of the form

$$\frac{\partial}{\partial t}(\rho\phi) + \text{div}(\rho\underline{u}\phi - \Gamma_{\phi}\text{grad}\phi) = S_{\phi} \quad (1)$$

where  $\phi$  stands for a generic fluid property and  $\rho$ ,  $\underline{u}$ ,  $\Gamma_{\phi}$ ,  $S_{\phi}$  are density, velocity vector, effective transport coefficient and source term, respectively. Pressure is calculated from a pressure correction equation deduced from the continuity equation ( $\phi = 1$ ) and the momentum equation ( $\phi = \underline{u}$ ).  $\Gamma_{\phi}$  is obtained from solutions for the turbulence kinetic energy ( $\phi = k$ ) and its dissipation ( $\phi = \epsilon$ ), with  $\Gamma_{\phi} = 0$  for  $\phi = 1$ ,  $\Gamma_{\phi} = \mu_{\text{eff}}$  for  $\phi = \underline{u}$ , and  $\Gamma_{\phi} = \mu_{\text{eff}}/\sigma_{\phi}$  for  $\phi = h, f, m_{fu}, k$  and  $\epsilon$ , where  $h$  is the enthalpy,  $f$  the mixture fraction, and  $m_{fu}$  the fuel mass fraction. Also  $\mu_{\text{eff}} \equiv \mu_t + \mu_t$ , where  $\mu_t$  is the molecular viscosity and

$$\mu_t = C_D \rho k^2 / \epsilon \quad (2)$$

where  $C_D$  is a model coefficient with a CFD standard value of 0.09.

In JASMINE the y coordinate is vertical and buoyancy appears in the source terms  $S_v$ ,  $S_k$ , and  $S_{\epsilon}$ . These are given in full in Cox and Kumar [2] and we will concentrate only on the contributions, from the buoyancy, denoted by  $S_{\phi,B}$ . These are:

$$S_{v,B} = -g(\rho - \rho_{ref}) \quad (3)$$

$$S_{k,B} = G_B = \mu_t g \frac{1}{\rho} \frac{\partial \rho}{\partial y} \quad (4)$$

$$S_{\epsilon,B} = C_1 \frac{\epsilon}{k} G_B \quad (5)$$

The mean pressure field is considered to be made up from a thermodynamic value set at around mid-height, a hydrostatic component which is a function of y only and corresponds to variation in a still column of fluid at an arbitrary density  $\rho_{ref}$ , and finally a hydrodynamic component p which arises from the fluid motion and density variations with height which differ from  $\rho_{ref}$ . The standard CFD value  $C_1 = 1.44$  is used [2].

The effects of buoyancy on turbulence generation and dissipation are often neglected, i.e.  $G_b = 0$  [17-19] or made more complex by varying the value of  $C_1$  depending on whether the buoyancy is stabilizing or unstabilizing [1, 20]. Chow and Leung [21] include low Reynolds effects into  $S_k$  and  $S_\epsilon$  for treatment of near wall flows but these do not modify  $G_b$  directly. Nam and Bill [22] use the JASMINE formulation for  $S_{k,B}$  and  $S_{\epsilon,B}$  but find that they need to double  $C_D$  to 0.18 and reduce  $\alpha_k$  to 0.85 (from standard value of 1.0) in order to fit the thermal plume data from large fires. (Note that for momentum driven jet diffusion flames  $C_D$  needs to be reduced below its standard value of 0.09 for round jets.) Most of the models claim to predict mean velocity and temperature in ceiling jet flows, some also the thermal part of the fire plume and few the burning part of the fire plume. Little attention appears to have been given to validation of the turbulence quantities predicted in these flows.

All in all, the situation with regard to modelling of buoyant flows is far from satisfactory. There are those who claim, e.g. [13], that the large scale structures present in buoyant plumes invalidate the gradient modelling approach of Eqn (1). They seem to contend that what is a sufficient condition (small eddies) for gradient modelling is a necessary condition. The recent work of Rogers and Moser [23] shows that even the two-dimensional mixing layer becomes fully turbulent when there are turbulent boundary layers at inlet and Rogers reports [24] that the turbulent transport obeys gradient modelling [25]. It may be that turbulent fire plumes cannot be satisfactorily modelled with a two-equation turbulence model of the  $k-\epsilon$  type. A full second-order closure may be necessary. It is, however, still worthwhile trying to improve the  $k-\epsilon$  modelling approach. For this a return to fundamentals is needed.

In the fire itself, and in the near field of the plume, density variations are large and the effects of density fluctuations cannot be neglected. The usual approach is to use density-weighted or Favre averaging [26, 27]. The density-weighted equations are still of the form of Eq (1) but the quantities  $\underline{u}$ ,  $f$ ,  $h$  are now recognized as density-weighted averages. Care must be taken with the source terms however. The buoyancy term in the turbulence kinetic energy equation is obtained [28] as

$$\begin{aligned}
 S_{k,B} &= - \overline{v'''} (\rho_{ref} g + \frac{\partial p}{\partial y}) \\
 &= \frac{\overline{\rho'v'}}{\rho} (\rho_{ref} g + \frac{\partial p}{\partial y})
 \end{aligned}
 \tag{6}$$

where the instantaneous velocity component  $\hat{v} = V + v' = \tilde{v} + v''$ , where  $V$  is the conventional average,  $\tilde{v}$  the density-weighted average

$$\tilde{v} \equiv \overline{\rho'v} / \rho
 \tag{7}$$

and  $v'$ ,  $v''$  the fluctuations from the conventional and density-weighted averages respectively. Here  $v = \tilde{v}$  as noted above and  $\rho$  is the conventional average of the density and  $\hat{\rho}$  its instantaneous value with  $\rho' = \hat{\rho} - \rho$ . Eqn (4) may be obtained from Eqn (6) by gradient modelling of  $\overline{\rho'v'}$ :

$$\overline{\rho'v'} = - \left( \frac{\mu_r}{\rho} \right) \frac{\partial \rho}{\partial y} \quad (8)$$

and making the Boussinesq approximation

$$\rho \approx \rho_{ref} \quad (9)$$

provided  $\rho_{ref}$  is chosen so that everywhere  $|\partial p/\partial y| < \rho_{ref} g$ . Remember that  $p$  in Eqn (6) is the pressure less its hydrostatic value. This term in Eqn (6) is usually neglected, but it only can be when  $\rho_{ref}$  is chosen as above.

In fire plumes both of the approximations (8) and (9) made in arriving at Eqn (4) from Eqn (6) are likely to be large sources of error. In the fire plume the vertical pressure gradient is given by the ambient hydrostatic gradient, which, if given by  $-\rho_{ref}g$ , results in an extra factor of  $\rho_{ref}/\rho$  being needed in Eqn (4). This can amount to a factor of 3 or 4 in the hot region of the fire. The flux modelled in (8) is a streamwise flux and gradient models do an extremely poor job for such fluxes. It is found for conserved scalars [25] that the major contribution to the streamwise flux comes from the transverse mean gradients acted on by the transverse momentum flux. In the far field of the plume where the specific volume behaves like a conserved scalar we obtain from [25]

$$-\overline{\rho'v'} \approx C_D \frac{k^2}{\epsilon} \left\{ a_1 \frac{\partial \rho}{\partial y} - a_2 C_D \frac{k}{\epsilon} \left( \frac{\partial v}{\partial x} \frac{\partial \rho}{\partial x} + \frac{\partial v}{\partial z} \frac{\partial \rho}{\partial z} \right) \right\} \quad (10)$$

where  $a_1$  and  $a_2$  are of order unity. In the near field of the plume the specific volume is affected strongly by both chemical reaction and radiant heat loss and the components of the density gradient change sign. Gradient modelling, even in the form of Eq (10), is unlikely to be useful. In the near field it may be necessary to solve a partial differential equation (pde) for  $\overline{\rho'v'}$ , as has been done by Kollmann [29,30].

In the ceiling jet the vertical component of the momentum equation assumes its boundary layer form so that

$$\frac{\partial}{\partial y} (p + \rho \widetilde{v'^2}) = -(\rho_{ref} - \rho)g \quad (11)$$

Eq (6) then becomes

$$S_{k,B} = \overline{\rho'v'} \left\{ g - \frac{1}{\rho} \frac{\partial}{\partial y} (\rho \widetilde{v'^2}) \right\} \quad (12)$$

The layer is stably stratified so that the density weighted vertical normal stress  $\rho v''^2$  is small. If variation in mean density across the layer is small the modelling of Eqn (4) will probably be adequate. Otherwise the effects of reaction and radiant loss on the modelling by Eqn (8) can be significant.

So far we have only considered the effects of buoyancy on  $k$  and  $\epsilon$ . Of far greater importance is the prospect that  $C_D$  will be affected directly and  $\sigma_\phi$  also for  $\phi = f, h, m_{fu}$ . Rodi [31, 32] uses Algebraic Stress Modelling (ASM) to obtain gradient models for the shear stresses and the scalar flux. The models include the effects of the mean scalar gradient on the shear stress and the mean velocity gradient on the scalar flux so that algebraic formula for  $C_D$  and  $\sigma_\phi$  do not result. Algebraic stress modelling of this sort is now proving useful in the modelling of meteorological flows, such as sea breeze fronts [31-33]. The analysis is only carried out for small variations in density and so would need modification for parts of the flow with strong density variations. It may be easier to go to a full second order closure than attempt to modify Rodi's [34, 35] analysis. For two-equation turbulence models it may be better to find a simple Richardson number dependence for  $C_D$  and  $\sigma_\phi$ .

Chemical reaction and its associated heat release can also affect gradient diffusion models [36]. In turbulent premixed flames the turbulent fluxes of scalars can be up the mean scalar gradient giving negative values for the turbulent diffusivity. For conserved scalars, such as the mixture fraction, it appears that the conventional modelling works quite well when density-weighted averaging is used. As yet there is no clear alternative available for reactive scalars, such as  $m_{fu}$ . Mixture fraction and enthalpy,  $h$ , are conserved under chemical reaction and gradient modelling should be satisfactory.

## CONVECTIVE HEAT TRANSFER

In fires the ceiling is usually far from adiabatic with conduction losses into the ceiling itself and radiant gains from the fire and losses to the room at large. Heat losses at the ceiling can be a substantial part of the overall heat balance. They may also be of significance for structural reasons and for fire penetration to the roof space or floor above.

Craft et al [37] show that the standard  $k$ - $\epsilon$  model does quite poorly in predicting the heat transfer near the stagnation point of a jet impinging on a flat surface in the absence of buoyancy effects. They provide an improved full second-order closure model which does much better. For the fire plume impinging on the ceiling, the effects of buoyancy will be quite complex. It is here that the flow changes from being unstable to essentially stably stratified. The performance of the  $k$ - $\epsilon$  model may appear to be quite good, albeit for the wrong reasons.

The ceiling jet is of course a stably stratified layer. For the most part! If the layer is being cooled from the top by heat abstraction at the ceiling through conduction and/or net radiation the boundary layer at the ceiling itself will be unstable unless the shear generated turbulence there is strong. The measurements of Motevalli and Marks [38] show the sudden drop in temperature at the ceiling surface. The situation is analogous to break-up of a ground-based inversion by solar heating in meteorology [33]. If the surface layer is unstable, greatly increased heat transfer can be expected. Numerical resolution of this thin

layer will be very expensive. Resolution of it to some degree is needed even if wall functions are to be applied.

Measurements of ceiling jets seem to pay little attention to the question of the effect of cooling (or heating) from the ceiling surface. Often insufficient information is given to make a reasonable judgement on this. Convective heat flux measurements are also difficult as the gauge is usually sensitive to radiation as well as convection. Furthermore, to get an accurate result the sensing surface should be at the same temperature as the surrounding surface. Otherwise a new thermal boundary layer with very steep temperature gradient is established at the gauge. Guard rings are of little help in this regard.

## COMBUSTION MODEL

JASMINE [2, 3] uses a version [18] of Spalding's [39] Eddy Break Up (EBU) model

$$R_{fu} = -\rho \frac{\epsilon}{k} \min[C_R m_{fu}, C_R \frac{m_{ox}}{s}, C'_R \frac{m_{pr}}{(1+s)}] \quad (13)$$

where  $R_{fu}$  is the mass consumption rate per unit volume of the fuel,  $m_{ox}$  and  $m_{pr}$  are the mass fractions of oxygen and products respectively and  $s$  is the mass ratio to stoichiometric of oxygen to fuel. Linear relationships hold between  $m_{ox}$  or  $m_{pr}$  and  $m_{fu}$  and  $f$ , and so they may be obtained without further pdes being solved. The coefficients  $C_R$  and  $C'_R$  are given empirical values of 2.0 and 4.0 respectively. Theoretical values [36] can be derived from fast chemistry conserved scalar theory [40] but show dependence on the form of the mixture fraction probability density function (pdf) that is assumed and the reactant mass fractions [41]. EBU modelling gives essentially the same result as is obtained using the presumed form pdf approach in which an equation for mixture fraction variance  $\tilde{f}^2$  is solved from its modelled pde, and the fast chemistry assumption is made [19, 20].

A major purpose of the combustion model is to provide the mean density  $\rho$  that is needed in the solution of Eqns (1). The enthalpy,  $h$ , is the so-called "standardized" enthalpy and includes the "chemical enthalpy" which may be denoted here as  $m_{fu} Q_c$ , where  $Q_c$  is the heat of combustion of the fuel. The sensible enthalpy is obtained as  $h - m_{fu} Q_c$  and this yields the temperature upon division by a suitable mean specific heat. The ideal gas law

$$P = \rho \frac{RT}{W_{mix}} \quad (14)$$

is then used to obtain  $\rho$ . Here  $P$  is the thermodynamic pressure (1 atm),  $R$  the universal gas constant and  $W_{mix}$  the mixture molecular weight given by

$$W_{mix}^{-1} = \sum_i \frac{m_i}{W_i} \quad (15)$$

The use of Eqn (14) neglects correlations of fluctuations. Since  $h$  and  $m_i$  are density-weighted averages it turns out that the neglect of these in this case gives only small errors of 1 or 2 per cent at most [42] for fuels with molecular weights near that of air. In the presumed-form pdf approach care must be used in evaluating the mean density since the pdf used is itself a density-weighted pdf and it must be used to average the instantaneous specific volume versus mixture fraction relationship [27, 40]. In non-adiabatic systems, such as fires, it would be better to use the pdf to calculate the mean fuel mass fraction and proceed as in the EBU approach above to find the temperature and then the density from Eqns (14) and (15).

Validation tests are often carried out with natural gas or an alcohol as the fuel. Practical fuels, such as plastics, wood, paper and liquid hydrocarbons, e.g. from spills, generate so much soot in their flames that radiation losses cause quenching and leave C, CO, hydrocarbons (HCs) and other unburnts in the plume. These unburnts affect the density of the fire plume in two ways:- by reducing the amount of heat released, and, by changing the emissivity and hence the amount of heat lost by radiation from the flames, the plume and the ceiling layer. Changing the ceiling layer temperature will also change the heat transferred into the ceiling by convection and conduction. Visibility in the plume and its toxicity are also important factors in fire modelling. Prediction of these species from fundamental kinetics is a daunting task beyond the scope of engineering fire models. Simpler methods are needed. Some effort is underway [4] to incorporate laminar flamelet modelling [43] into JASMINE for this purpose. This may give satisfactory predictions of species within the flame but it is not clear how this approach will yield worthwhile predictions of the quenched emissions from the fire. A simpler, more empirical approach is needed, at least for the time being.

For well-ventilated fires, i.e. well before flashover, using empirical emission indices  $E_i$  for the species  $i$  in the plume just beyond the flame tip gives a practical conceptual basis. The  $E_i$  are defined per unit mass of fuel gasified so that

$$m_i = E_i f \quad (16)$$

Empirical correlations for the  $E_i$  dependent on fuel type, fire size, fire type (pool, wall, corner) can be developed from full-scale fire data and bench scale test apparatus such as the cone calorimeter. Tewarson [44] and Köylü & Faeth [45] provide data of this type, but it has been obtained in small scale experiments. The effects of vitiation of the air entrained into the flaming region may also be included in the correlations. Some care will, however, be needed in defining vitiation and obtaining a suitably averaged value for the flaming zone, since the  $E_i$  will not be functions of space in the near field. (In the far field they could be back-dated for flow time from the flame zone and corrected for deposition on walls, etc.). Temperatures may be obtained from

$$\bar{c}_p T = h - \sum_i m_i Q_i \quad (17)$$

where  $Q_i$  is the heat of combustion for species  $i$ , being zero for  $O_2$ ,  $CO_2$ ,  $H_2O$  and such species as HCl. Density is then obtained from Eqns (14) and (15) as before. Where condensation of species occurs, such as for  $H_2O$  and tar, appropriate equilibrium



relationships will probably suffice to determine the proportion of  $E_i$  in each phase with  $Q_i$  in Eqn (17) being adjusted accordingly. For fires in which considerable pyrolysis occurs from unignited sources such as walls and other items of furniture a similar approach may be used by defining  $F_i$  as the "emission" index for pyrolyzate so that

$$m_i = F_i m_{fu} + E_i f \quad (18)$$

Tewarson [44] also provides data for  $F_i$  for some fuels.

A similar approach is often taken for the heat lost from the flaming region by radiation. In Eqn (17) this amounts to setting

$$h = c_{p,air} T_{air} + \eta Q_c f \quad (19)$$

where subscript air refers to values in the inlet air and  $1 - \eta$  is the fraction of the heat release that is lost by radiation. This approach can work well for zone models [6] or field models in which the radiation is not coupled to the gas phase. More advanced field models use flux [46] or discrete transfer [47] models for radiation which are fully coupled to the gas and the global approach of (19) is not appropriate. It is also evident that vitiation of the air makes for difficulties in the approach embodied in Eqn (19).

Where the radiation model is coupled to the gas phase, estimates are needed of the gas composition and the soot volume fraction  $f_v$  in the flame region. For engineering models these can be taken to be functions of mean mixture fraction as correlated from experimental data, with values suitably averaged over the fire volume. Alternatively instantaneous "state relationships" [48] for soot mass fraction as a function of instantaneous mixture fraction may be used and weighted by the mixture fraction pdf. This requires the availability of the mixture fraction variance  $f''^2$  solved for from its own pde. This approach has a lot of appeal as it is known [48] that the soot is present in high concentrations in only a narrow band of mixture fraction on the rich side of the flame. Instantaneous measurements of mixture fraction are, however, difficult in the rich part of turbulent diffusion flames and it is doubtful that the soot data from laminar flames will be appropriate. A further alternative is to solve a separate pde for the soot volume fraction with appropriately modelled production and consumption terms [18, 49].

As the fire grows toward flashover the use of empirical data from free-burning fires becomes less and less justifiable. The flame zone is less cooled by radiant loss giving less emission of unburnts. Ignition of fuel plumes from pyrolysing "targets", such as furniture and wall panels, becomes important as does the ignition of pyrolyzate fuel and unburnts in the ceiling layer [50]. A capability for calculating such phenomena will improve the versatility of the model even if the initial fire growth on a single object is taken as specified as a function of time. Piloted ignition (by sparks) can perhaps be assumed and ignition criteria specified in terms of temperature and mass fractions of unburnts and fuel pyrolyzate [51]. Note that for pyrolysing (and burning!) fuel surfaces the mixture fraction at the surface is much less than unity, it being determined by the gasification rate and the rate of turbulent convection. Propagation of the ignition could be left to the EBU model with a global kinetic rate perhaps being used to limit propagation into regions which are

too fuel-lean and to cause extinction of premature ignitions of the ceiling layer.

For the under-ventilated fire which exists after flash-over, very high concentrations of CO are present in the fire compartment and are not completely burned on mixing with air in the exit flow. These emissions represent a very considerable hazard in many fires. The available data [52] indicate that unburnt fuel remains with the CO so that assuming chemical equilibrium for the rich products will give too much CO and temperatures which are too low. Laminar flamelet models [43] will also not be effective. An EBU model based on one-step kinetics will not give CO but an EBU model [53] based on the 4-step reduced mechanism [54] may be useable.

Advanced methods of modelling turbulence combustion interactions are available, such as Monte Carlo joint pdf methods [55] and conditional moment closure (CMC) methods [56-59]. As yet they have not been used to address the problems present in fires, such as extinction by radiation cooling and chemistry in under-ventilated enclosure fires. It is expected that they will be able to give adequate predictions for these problems but the methods are likely to be computationally intensive and not practical for general field model codes within this decade. They do have a place in research, however.

## DISCUSSION

It can be seen that a field model for fires contains a large set of complex interacting submodels. Only a few of these submodels have been considered here. Others not addressed include radiant emissivity, effects of turbulent fluctuations on radiant emission and absorption, wall functions for friction and heat transfer, boundary conditions at flow inlet and exit, and numerical methods. Erroneous treatment of these submodels can lead to substantial errors. Erroneous treatment of several of them can lead to no error at all! This will happen if the errors compensate one another for the test variable under scrutiny in an overall evaluation. Are we sure we don't get the right answer because we stop our debugging and submodel upgrading when prediction and experiment match? May not there be many more errors to find and submodel upgrades needed? And might not these change substantially other aspects of the results, such as radiant heat flux to the floor, and yet leave the "validation" variable (e.g. temperature in the exhaust flow) unchanged? And may erroneous answers be obtained when the geometry and/or other conditions are changed significantly? It is obvious that a code developed to use  $C_D = 0.18$  to get good predictions for buoyant fires, will do poorly on fires fueled by a jet of fuel unless there is an appropriate submodel for the effect of Richardson number on  $C_D$ . How sensitive are the results to the boundary conditions used? Will different users of the code get the same results on the same problem?

From the viewpoint of quality control and quality assurance it is clear that field models need to be able to demonstrate a documented pedigree validating all of the submodels involved in the problem. They must first of all be grounded in good physics and maintain their links to CFD and furnace modelling by only changing turbulence models and radiation models in ways which can be thoroughly justified. A hierarchy of well-documented and well-vetted experimental data on buoyant flows and fires needs to be established. These should have detailed information on boundary conditions and comprehensive measurements of mean values of composition, temperature, velocity and

heat flux and of turbulence quantities, such as  $k$  and rms temperature fluctuations. For any application, a fire field code needs to demonstrate that it has performed satisfactorily on the appropriate subject of this overall hierarchy which is relevant to the problem in hand and with the submodels and coefficients that are to be used on the problem in hand. It should quantify what is meant by "satisfactory" performance. This pedigree can be used in training and validating new users of the code.

Since a great amount of detail is available, field models can provide information which can be used to establish credibility for the model in other ways. For example, where a fully coupled radiation model is used, an integration over the flaming region or over the total plume can be used to report on the heat loss fraction due to radiation so that this may be compared with any data available for this or similar fuels. Detailed mass and energy balances can be given; and the flame height and heat flux at the plume impingement point can be compared with that given by empirical correlations. Mass flow rates through openings and for air entrainment into the plume can also be compared with empirical formulae. It is a relatively simple matter to provide such information as part of the output from the code.

Increased use of field models in fire science investigations will not only improve experimental techniques and theoretical understanding of fire problems, it will also improve the field models and their credibility among fire engineers. Research directed directly at improving submodels, such as for chemistry in under-ventilated fires, is also needed.

At this stage of their development field models can only be used qualitatively in fire safety engineering. With quality assurance procedures developed so that well-documented pedigrees of validation are provided and users properly trained the models should soon be available for use in a semi-quantitative way. Just as zone models should also be used in a semi-quantitative way. Allowance must be made for the uncertainties in the modelling in both cases. My expectation is that in five years the field model will give much more credible results for many problems of interest to fire safety engineers and will be in widespread use in the profession.

## CONCLUSIONS

The submodels used to incorporate the effects of buoyancy on turbulent transport of momentum and species have been considered in some detail and needed improvements identified. Correct derivation identifies a factor  $\rho_{ref}/\rho$  missing from the buoyancy generation term used in the  $k$  and  $\epsilon$  equations. The gradient model used in this term also needs improvement for the plume part of the flow. A Richardson number dependence for the coefficient  $C_D$  in the turbulence flux model is needed, although full second order closure may be necessary in the long term.

For convective heat transfer, improvements are needed for the heat transfer at the point of plume impingement on the ceiling and for including the effect of the unstable layer above the stable layer in the ceiling jet when the ceiling is cooling the jet.

The care that is needed in formulating combustion models and the way in which they are

used to obtain the mean density has been surveyed, paying particular attention to the fact that density-weighted averaging is implicit in the equations being solved. The formulation of semi-empirical models for handling the contributions of minor species in the flaming region of the fire plume and in the overfire region is canvassed so that their effects on density and radiant emissivity can be properly included.

In order to establish quality assurance it is necessary for field models to have a well-documented pedigree of validation for all the submodels involved. The selection of an heirarchy of well-vetted and well-documented experiments to be used for this purpose is recommended. In this way the credibility of field models will be established and it is expected that in five years they will largely have surpassed the use of zone models by professional fire safety engineers.

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