SOME RECENT PROGRESS IN THE FIELD MODELLING OF FIRE

G COX
(Fire Research Station, Borehamwood, Hertfordshire, WD6 2BL, UK)

ABSTRACT

Mathematical field models that calculate the movement of smoke within enclosures have now matured to the point at which they are enjoying increasing application particularly to practical building design. This represents just one of two distinct branches of active development in the use of computational fluid dynamics for fire problems.

The detailed modelling of combustion in buoyant turbulent diffusion flames also remains an important research objective. Whilst current capabilities may be adequate for the modelling of far-field applications, improved treatments are needed to reliably predict chemical species yield in underventilated fires and to fully couple thermal radiation fields to solid phase pyrolysis.

This paper briefly reviews progress in the field modelling of fire. Examples of recent application and development work are used to illustrate current capabilities and suggestions made as to where further work is needed.

INTRODUCTION

Computational fluid dynamics has made an increasingly significant contribution to many branches of engineering since its emergence in the mid 1970's as a practical design and analysis tool. Examples of its application can be found in many areas of endeavour ranging from airframe, ship hull and car body design through to analyses of the efficiency of gas turbines, cement kilns and glass furnaces.

By solving, numerically, the full partial differential equation set describing the principles of local conservation of mass, momentum, energy and species, subject to the particular boundary conditions of the problem, models of this type have enjoyed widespread development in many combustion applications. Until comparatively recently, however, their use in fire research has been limited, tending to concentrate more on validation of the methodology than on its development and application.

A growing confidence in predicting far-field conditions gained from these studies, in addition to the availability of increasing computer power at reducing cost, has encouraged greater interest in their use for the assessment and design of smoke control systems in buildings.

This represents, however, just one of two distinct branches of active development of field modelling, as it has become known in fire science. The detailed modelling of turbulent buoyant diffusion flames, particularly in underventilated conditions, and the full coupling of the thermal radiation field to the rate of gasification of solid fuels also remain important areas of active research and development.

This paper provides a brief review of recent progress in both the application and development of field modelling.

GOVERNING EQUATIONS

Computational fluid dynamics models start with the 'exact' instantaneous partial differential equation set describing local conservation principles. These are then solved subject to the following critical decisions:

(a) how to treat the problem of turbulent closure

(b) which algorithm is to be used to calculate the numerical solution of these equations at interior points of the flow domain

(c) how to properly approximate boundary conditions along the domain boundaries and

(d) how to treat specific combustion chemistry or multi-phase flows.

The basic equation set for the simulation of fires in enclosures comprises time-averaged conservation equations for mass, momentum, energy and chemical species of the general form

$$\frac{\partial(\rho\phi)}{\partial t} + \frac{\partial(\rho u_i \phi)}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\Gamma_\phi \frac{\partial \phi}{\partial x_i}\right) = S_\phi \qquad (1)$$

[time rate of change] [convection] [diffusion] [source/sink]

where ϕ is the generic variable which may represent the three Cartesian velocity components u_i, the enthalpy h or the mass fraction of a particular species m_j. (The mass continuity equation is represented by the case $\phi = 1$). S_ϕ is a source term appropriate to ϕ which incorporates, for example, the effects of chemical production and radiative heat loss. A fuller description specifically in relation to enclosure fires is given by Cox and Kumar[1].

All dependent variables in equation (1) are time-averaged quantities and, since density fluctuations have been neglected, may be viewed as implicitly density-weighted, for example,

$$u_i = \frac{\overline{\rho u_i}}{\bar{\rho}} \; .$$

The diffusion term incorporates the effects of both turbulent and molecular diffusion through the exchange coefficient Γ_ϕ. In most field modelling studies of fire it has been assumed that the Reynolds stresses and scalar fluxes, which involve the correlations of fluctuating properties, can be modelled by use of the gradient transport hypothesis, which for scalars is

$$\overline{\rho u_i' \phi'} = - \Gamma_\phi \frac{\partial \bar{\phi}}{\partial x_i}$$

To determine the local value of Γ_ϕ, two further transport equations are solved for k, the turbulence kinetic energy and ε its rate of dissipation. The effects of buoyancy on extra turbulence production (in rising plumes) and inhibition (in stratified layers) require special attention[2].

The modelled conservation equations are then discretised and solved iteratively using the SIMPLE procedure[3] or one of its variants.

Solution of these equations alone, together with the appropriate boundary conditions to incorporate the effects of heat and momentum loss to the enveloping structure, is sufficient to capture the major features of the smoke movement problem[4] for a known fire size. It does not however provide a framework to address the critical issues of fire growth or the production and spread of the incapacitating products of combustion, both gaseous and particulate.

For this combustion and radiation "sub-models" are required to allow assessments to be made of the hazard to human life due to inhalation of toxic gases and to radiant and convective heat exposure.

COMBUSTION CHEMISTRY

The treatment of the effects of turbulent transport has already been discussed briefly. Unfortunately the turbulent mixing process also has a significant influence on the mean rate of chemical reaction. The hydrodynamic mixing of fuel with air is much slower in fires than is their rate of reaction and so it is this which controls the rate of fuel 'disappearance', R_{fu}, or of product yield.

A simple method for dealing with this difficulty is to allow the combustion to be controlled only by the rate of small scale turbulent mixing between the reactants and for that rate to be further controlled by the concentration of deficient reactant. In air-rich locations, reaction is controlled by lack of fuel and vice-versa in fuel-rich locations, thus

$$R_{fu} = - \frac{C \rho \varepsilon}{k} \left[m_{fu}, \frac{m_{ox}}{s} \right]_{min}$$

where m_{fu}, m_{ox} are the local mass fractions of fuel and air, s is the stoichiometric ratio and C is a numerical constant.

A transport equation for m_{fu}, incorporating the above source term, is solved in addition to one for the normalised mixture fraction, f, where

$$f = \frac{\left(m_{fu} - \frac{m_{ox}}{s} \right) + \frac{m_{ox,\infty}}{s}}{m_{fu,o} + \frac{m_{ox,\infty}}{s}}$$

which is simply conserved and does not therefore involve a source term. (The subscripts (o,∞) denote conditions in the fuel supply and ambient air respectively). This method has been reasonably successful[1,5] in predicting the major features of a wide range of building fire problems including the stable species of CO_2 and H_2O. Models containing this simplistic treatment of combustion chemistry are now being used as application tools to assess a variety of smoke movement problems. This is exemplified by two recent applications.

Fig 1 shows an example of an application[6] of the JASMINE model[1] to the assessment of smoke control provision in a very large atrium (~500,000m³). Predictions are shown of visibility contours (empirically related to product mass fraction), on a vertical plane through the main atrium, resulting from a growing 'design' fire at its base.

The plume rises naturally against an initial ambient temperature gradient of 25°C between floor and ceiling. At 65 secs the plume is calculated to be detected at first floor level, causing extraction fans at the ceiling to operate. Replacement air supplied at low level from opposite ends of the atrium causes the plume to be deflected over the floor (and occupants) until the increasing buoyancy of the growing fire restores the plume to rise normally by about 10 minutes.

Field modelling of this type also made an important contribution to the formal investigation[7] of the King's Cross underground fire that occurred in London in 1987. This fire, which killed 31 people, occurred on an escalator adjoining the main ticket hall of the underground railway station. The modelling suggested a mechanism to explain the rapid fire development that had not been considered by the fire investigators. Quite simply it showed that the plume from a fire occupying the full width of an escalator channel, instead of rising vertically, would attach to its base, laying in the channel and thus in intimate contact with the wooden floor treads and side panels.

Fig 2 shows predictions of gas temperature for two situations[8]. Early in the fire, when it has yet to spread across the full width of the channel, the products of combustion rise vertically to impinge and to move upwards underneath the ceiling of the enclosing tunnel. Later, when the fire has spread across its width, the plume of products drops into the channel not rising to the ceiling at all.

Chemical kinetics however have played little part in modelling of this kind. To determine the levels of toxic intermediates such as CO and to predict soot formation, a prerequisite to the accurate prediction of luminous radiation from flames, a more realistic treatment for finite rate kinetics is required.

If the balance equation for mean mixture fraction, $\bar{f}$, is complemented by a further equation, of the form of equation (1), for its variance, $\bar{f'^2}$, then the turbulent scalar mixing field can be characterised by a local probability density function, controlled by these two moments.

The modelling task then concerns the relationship between instantaneous species concentrations and the mixture fraction, which characterises the turbulent mixing field. The simplest such relationship assumes full local chemical equilibrium. However this assumption is not generally valid within the flame and substantial errors in estimating the yield of such intermediates as CO can result.

An alternative approach currently under development for application to fires is the laminar flamelet model[9]. Burning in a turbulent flame is here assumed to occur locally in laminar-like flamelets. The relationship between species compositions and mixture fraction in such circumstances can be determined entirely computationally for

simple fuels such as methane or propane, for which the chemistry is sufficiently well understood. More importantly however it can also be determined 'once and for all', by experimental measurement in well controlled laminar flames for the fuels likely to be encountered in practical fire problems[10]. These 'state relationships' can be stored in a 'library' for access by the hydrodynamic calculation for the determination of detailed gas species. This approach is currently being developed for detailed modelling of both well and poorly ventilated fire sources.

Fig 3 shows a comparison of laminar flamelet calculations[11] with measurements on the axis of a 18 kW methane-fueled fire simulation on a 0.3 m square burner. The reasonably good agreement shown by the figure belies a difficulty in selecting appropriate source boundary conditions for buoyant fires. The flow immediately above the burner undergoes a laminar-turbulent transition which has not yet been treated satisfactorily by the turbulence model. To obviate this problem the calculations shown in figure 3 were initiated 85 mm from the burner using experimental measurements for mean velocity and temperature, k, ε, $\bar{f}$ and $\overline{f'^2}$. Although this difficulty does not present serious problems to far-field modelling it needs to be resolved for the accurate treatment of the near field. Baum et al[12] have recognised this difficulty with turbulence modelling and instead directly solve inviscid approximations to the transport equations capturing the energy-containing low frequency eddies without attempting to model, at sub-grid scale, viscous stress and thermal conduction effects.

With sufficient knowledge of the appropriate boundary conditions above the transition, as in the calculations presented in figure 3, the gradient transport closure has been extended to the prediction of soot volume fraction using a semi-empirical model for soot formation[13]. The processes of soot nucleation, surface growth and agglomeration can be represented by rate constants also determined by local mixture fraction and temperature.

THERMAL RADIATION

Two quite distinct difficulties need to be addressed for the realistic modelling of radiant heat transfer. The first concerns 'geometrical' problems associated with the exchange of radiant energy between remote emitters and receivers, be they solid surfaces such as walls or particulate/gas phase mixtures such as flames. The second difficulty concerns the calculation of local emissive power. The relative contributions from broadband soot and banded gaseous emissions will vary substantially between flame and smoke products. In addition, as with transport processes and combustion chemistry, the effect of turbulent fluctuations in temperature and gas composition must be considered, particularly at the fire source itself[14].

Both flux[15] and discrete transfer methods[16] have been used in conjunction with predictions of time-mean temperature and composition fields for enclosure fire simulations. More comprehensive treatments of thermal radiation which include the interaction effects of turbulent fluctuations by exploitation of the laminar flamelet treatment for combustion have to date been restricted to the fire source alone and again only for comparatively simple hydrocarbon fuels.

Fig 4 illustrates detailed radiative predictions for a methane fuelled fire simulation, identifying the significant contribution made by turbulent fluctuations in scalar properties in the flame.

SOLID PHASE

It is in the coupling of the gas and solid phases where field treatments tend to converge with the zonal fire modelling philosophy. Field models can in principle

extend their numerical solutions of the conservation equations into the solid boundaries. Whilst this is useful for determining the heat lost from the gas phase, by conduction into the structure, it is unlikely to be of much practical value for the calculation of rates of heat release or flame spread over flammable solid fuels for anything other than the simplest of materials. Those used in practice for furnishings and upholstery tend to be laminates and composites, which under fire conditions may melt, char or delaminate - all poorly understood processes at the level of detail necessary.

In a field model treatment for the burning of wooden cribs, Fan and Wang[17] did use empirical expressions relating mass pyrolysis rate to calculated fuel surface temperature. However, more generally a pragmatic approach is required. Quintiere[18] has developed a model for flame spread which is based upon the measurement of material properties under 'fire conditions' in a standardised small scale fire test. These are simply a critical heat flux for piloted ignition together with a flame spread coefficient related to the thermal properties of the material.

With such measurements, gas phase models can be used to provide the appropriate surface boundary conditions to translate performance in a standard fire test to actual in-fire behaviour. A recent paper by Opstad[19] has shown how the results from cone calorimeter measurements can be exploited along with an assumed surface ignition temperature within a field model to produce predictions of flame spread. This synergy between mathematical modelling and standard testing is likely to grow such that in future more meaningful appraisals can be made of fire hazard than those based on existing reaction-to-fire test methods.

WATER DROPLETS

Sprinklers are used routinely to protect buildings against the rapid growth of fire. These are based on the simple principle that applying water to burning fuel and potential fuel ahead of a fire will limit its growth. The proper design of such a system requires careful consideration however since the interaction of a spray with the products of combustion is extremely complex. The spray itself can entrain air and combustion products thus bringing smoke down to low level. Furthermore if droplets have insufficient downward momentum they can be lifted by the buoyant plume and indeed evaporate without having the opportunity to extinguish the fire.

There has been an increased interest in the use of water sprays for controlling fires partly to satisfy the need to develop novel on-board fire protection systems for aircraft and partly to find environmentally acceptable replacements for halon extinguishants.

The field modelling approach has been extended to apply to such problems[20,21]. By introducing extra contributions describing interphase transfer into the source terms of the gas phase conservation equations and by solving additional equations of motion for the droplets it is possible to trace their trajectories, size and temperature histories as well as their effect on the gas phase. An illustration is given in figure 5. Here a representative line of droplets is injected into a compartment containing a 400 kW pool fire at the centre of its floor. With the 0.5 mm droplets chosen, very few reach the floor with most being lifted and evaporating near the ceiling. With 1 mm droplets, not shown, all reach the floor. The availability of increasingly more powerful computer hardware is encouraging further development of this approach following progress elsewhere in combustion research in the modelling of fuel sprays.

CONCLUSIONS

In this brief review of progress in field modelling examples have been used to illustrate some current applications and developments. Although it has not been

possible to give a comprehensive review in the space available it is hoped that the reference list will assist the reader in locating relevant work.

Whilst reasonable validation can be demonstrated for far-field conditions there are often too few detailed comprehensive measurements particularly of the near-field to adequately test the full details of this modelling approach. The particular treatments required for the effects of turbulence on combustion chemistry and thermal radiation need further development and testing. Work will also continue to improve the accuracy of the numerical algorithms exploited (eg Morita et al[22]).

In some respects theoretical developments have outstripped the ability of traditional compartment fire experimentation to supply the underlying data needed. Because field modelling provides a very detailed prediction of property fields it creates a severe demand on experimentation. Measurements that may be satisfactory for testing zonal models are inadequate for testing field models. There is a growing need to meet this demand for the measurement of local flow velocities, product concentrations and radiative fluxes with modern diagnostic methods that have already contributed significantly to other areas of combustion-related research.

REFERENCES

1. Cox G and Kumar S. Field Modelling of Fire in Forced Ventilated Enclosures, Combustion Science and Technology 52, 7, 1987.

2. Markatos N C, Malin M R and Cox G, Mathematical Modelling of Buoyancy Induced Smoke Flow in Enclosures. Int J Heat Mass Transfer 25, 63, 1982.

3. Patankar S V and Spalding D B. A Calculation Procedure for Heat, Mass and Momentum Transfer, in Three-Dimensional Parabolic Flows. Int J Heat Mass Transfer 15, 1787, 1972.

4. Satoh K and Kuwahara, A Numerical Study of Window-to-Windov Propagation in High-Rise-Building Fires, p355, Proc Third International Symposium on Fire Safety Science, Elsevier, 1991.

5. Cox G, Kumar S and Markatos N C. Some Field Model Validation Studies, Proc First Intl Symp on Fire Safety Science p 159, Hemisphere 1986.

6. Cox G, Kumar S, Cumber P, Thomson V and Porter A. Fire Simulation in the Design Evaluation Process, Proc Interflam 90, p56 Interscience 1990.

7. Fennell D. Investigation into the King's Cross Underground Fire, Her Majesty's Stationery Office, London 1988.

8. Cox G, Chitty R and Kumar S. Fire Modelling and the King's Cross Fire Investigation, Fire Safety Journal 15, 103, 1989.

9. Liew S K, Bray K N C and Moss J B. A Stretched Laminar Flamelet Model of Turbulent Non-Premixed Combustion. Comb. and Flame, 45, 199, 1984.

10. Moss J B, Cox G and Kumar S. 'Laminar Flamelet Models of Fire - the Prospect', p53, Fundamental Aspects of Polymer Flammability, Institute of Physics, Bristol, 1987.

11. Syed K J and Moss J B. Flamelet Modelling of Species Concentration in Fires, Cranfield Institute of Technology, Private Communcation 1991.

12. Baum H R, Rehm R G, and Mulholland G W. Prediction of Heat and Smoke Movement in Enclosure Fires, Fire Safety Journal, 6, 193, 1983.

13. Syed K J and Moss J B. Modelling Thermal Radiation from Buoyant Fires. School of Mech. Eng Report 88/1, Cranfield Institute of Technology, 1988.

14. Cox G. On Radiant Heat Transfer from Turbulent Flames, Comb. Sci and Tech. 17, 75 (1977).

15. Kumar S and Cox G. Mathematical Modelling of Fire in Road Tunnels - Effects of Radiant Heat and Surface Roughness, Transport and Road Research Laboratory, Contractor Report No 101, 1988.

16. Lockwood F C and Malalasekera W M G. Fire Computation: The Flashover Phenomenon, Proc 22nd Symposium (International) on Combustion p1319, The Combustion Institute 1989.

17. Fan W and Wang J. Predictions of Unsteady Burning of a Fuel Bed, p325, Proc Third Intl. Symposium on Fire Safety Science, Elsevier 1991.

18. Quintiere J G. A Simplified Theory for Generalising Results from A Radiant Panel Rate of Flame Spread Apparatus, Fire and Materials, 5, 52, 1981.

19. Opstad K. Fire Modelling using Cone Calorimeter Results, Proc First Intl. EURIFIC Seminar, p65, Interscience, 1991.

20. Ayers W H. Private Communication 1986.

21. Chow W K and Fong N K. Numerical Studies on the Sprinkler Fire Interaction Using Field Modelling Techniques, Proc. Interflam 90, p25, Interscience, 1990.

22. Morita M, Oka Y and Hirota M. Numerical Analysis and Computational Methods of Heat Flow in Fire Compartment p189, Proc Second International Symposium on Fire Safety Science, Hemisphere, 1989.

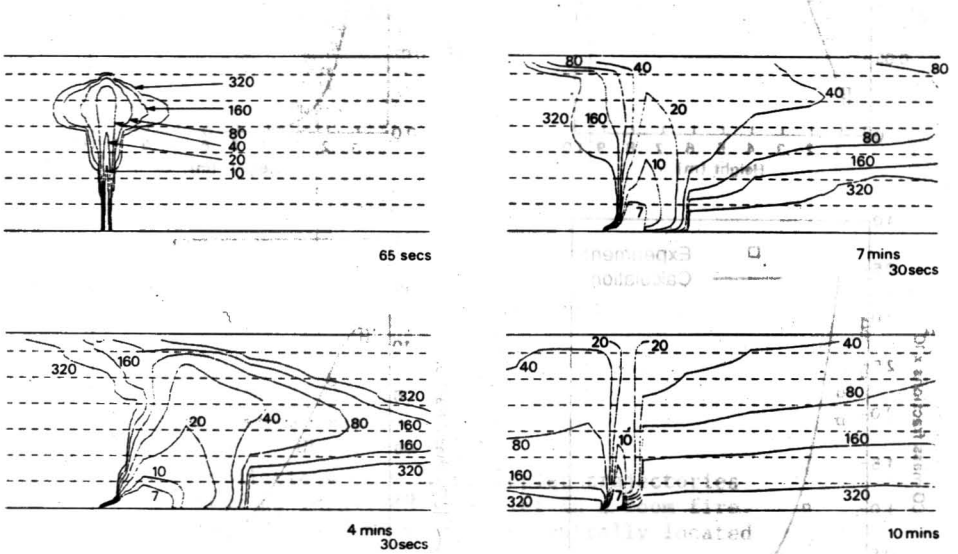


Fig 1. Evolution of smoke 'visibility' contours (m) on section through a large atrium

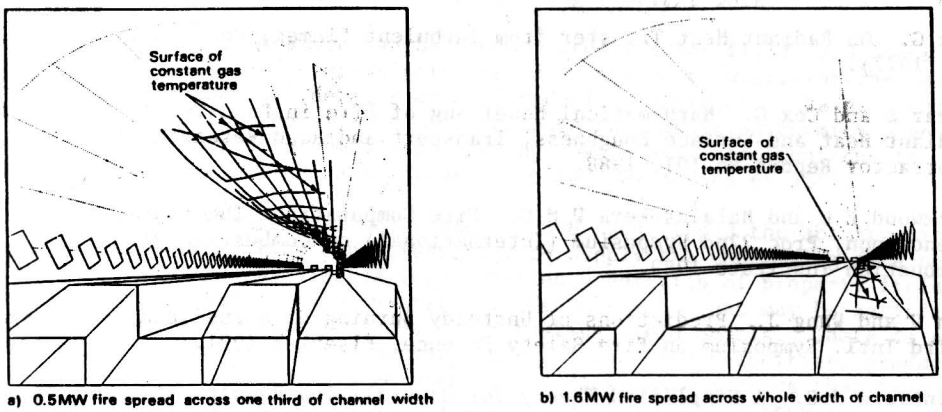


Fig 2. Predicted gas temperature surface of 50°C in King's Cross fire

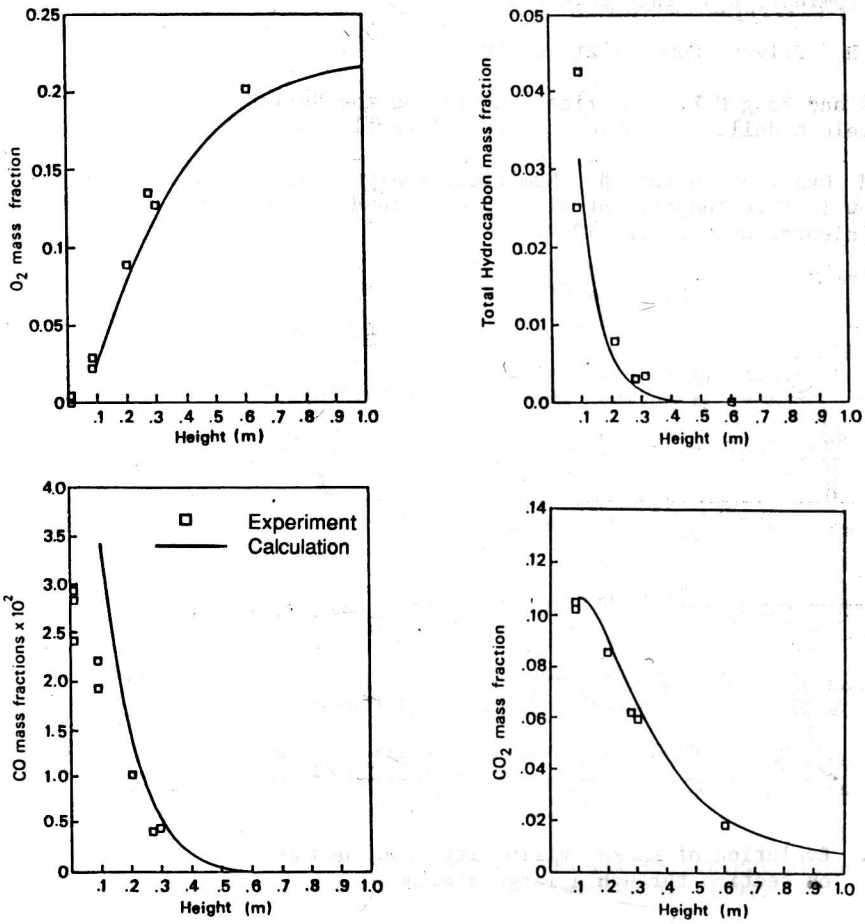


Fig 3. Laminar flamelet calculations and measurements in 18 kW methane fire simulation

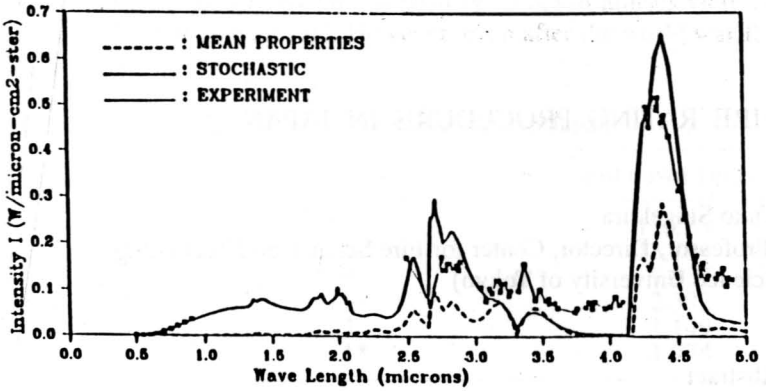
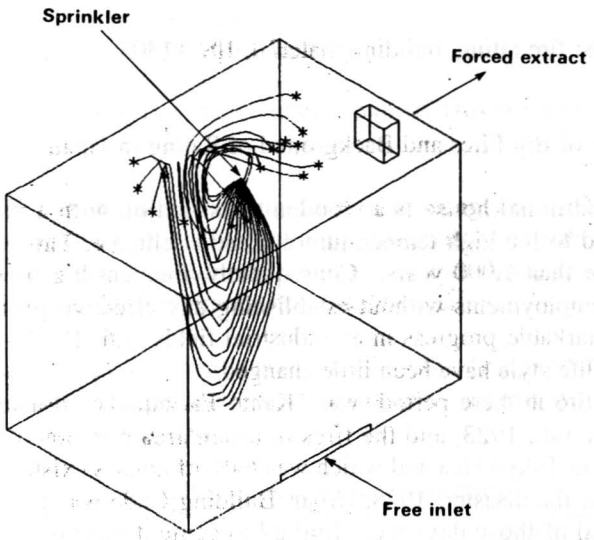


Fig 4. Spectral intensity for line-of-sight through methane fire simulation (0.14 m from burner)



* Represents total evaporation

Fig 5. Predictions of 0.5 mm droplet trajectories from an idealised sprinkler in a room fire. The 400 kW fire source is centrally located