

Coupled Soot and Radiation Calculations in a Compartment Fire

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ABSTRACT

A strategy is described in which an extended flamelet approach to soot modelling is linked to the discrete transfer radiation model, incorporating a weighted sum of grey gases solution to the radiative transfer equation. The simplification to chemical source term representation during turbulent burning, which is introduced by laminar flamelet modelling, is applied to a reduced description of soot formation. Into a standard eddy break-up combustion model, two additional scalar balance equations are introduced for the soot volume fraction and its number density. The influence of localised heat loss due to thermal radiation on the processes of nucleation, coagulation and surface growth is then incorporated through multiple flamelet state relationships, distinguished from each other by the extent of heat loss. Radiation properties, emissivities and intensities, are computed from local mean values of state variables (concentrations of CO₂, H₂O and soot) and temperature is evaluated from the enthalpy balance equation incorporating radiative exchange. The approach is implemented in the fire-specific CFD code, SOFIE, developed at Cranfield, and demonstrated in a jet flame for which extensive experimental property maps are available and in a representative compartment fire prediction.

INTRODUCTION

Radiative heat transfer is a significant contributor in the majority of flame spread mechanisms. Consequently a prerequisite to the accurate numerical simulation of flame spread and the accompanying fire growth must be an accurate numerical simulation of the radiative heat transfer to the combustible surface itself. This requires, in general, knowledge of both the local gas temperature, species concentrations and, most importantly in fires, the local soot volume fraction.

Unfortunately progress in the representation of increasingly complex combustion chemistry in computational fluid dynamics (CFD field model) predictions of turbulent burning in building fires has also exposed significant shortcomings in the accompanying models of soot formation and radiative heat transfer. To date, essentially ad hoc representations of radiative heat loss have been employed in detailed predictions of turbulent flames - for example, in the form of perturbed state relationships, incorporated in fast chemistry/conserved scalar combustion models [1,2], or approximate descriptions of radiative flux in the optically thin limit, introduced into the balance equation for mean mixture enthalpy [3,4] - but these admit only limited practical application. Indeed, in the simulation of room fires, radiation heat

transfer is usually incorporated within the framework of quite rudimentary representations of combustion chemistry.

The comparatively slow chemistry of soot formation requires that additional balance equations be solved for soot properties, whilst their strong temperature dependence necessitates that the influence of turbulent fluctuations also be accommodated in their averaged forms. The processes of soot formation and associated radiative heat loss are therefore closely coupled.

The present study therefore develops a methodology which incorporates a multiple laminar flamelet based description of soot formation in which families of soot source terms, expressed as functions of mixture fraction, are distinguished by the degree of radiative loss experienced and averaged over the mixture fraction *pdf* [5]. Heat release is accounted for using either an eddy break-up or laminar flamelet combustion model, coupling to a radiative heat transfer simulation using the discrete transfer method within an elliptic flowfield calculation. Whilst turbulent fluctuations are accounted for within the laminar flamelet description, turbulence/radiation interaction has, at this time, been described using mean values only of temperature and species concentrations.

Validation of the underlying flowfield simulations obtained using **SOFIE** have previously been published [6]. In this paper the coupled solution methodology is initially validated by detailed comparison between the CFD predictions and experimental measurements in a laboratory scale methane fuelled jet flame. In the absence of comparably detailed property measurements in compartment fires, a demonstration calculation is then presented for a simulated 600kW pool fire centrally located within a 2.8m square room with a single doorway open to the atmosphere, illustrated in figures 3 and 4.

NUMERICAL MODEL

The numerical simulations were carried out using the code **SOFIE** (Simulation of Fires in Enclosures), specifically developed at Cranfield for compartment fire predictions. **SOFIE** is based upon a finite volume procedure utilising an underlying general non-orthogonal coordinate system with co-located velocities, momentum smoothing and a pressure correction algorithm. Dependent variable interpolation is achieved using either a first order scheme (Hybrid or Power Law) or a TVD based second order accurate scheme. Turbulent closure is effected through a two equation, k- ϵ model incorporating buoyancy modifications [7].

Combustion

The principal heat release model is based upon the eddy breakup [8] concept in which it is assumed that the chemistry is fast and therefore turbulent mixing is rate controlling, according to the turbulence time scale, k/ϵ , such that the mass rate of fuel consumption may be written

$$R_{FU} = \bar{\rho} \frac{\epsilon}{k} \min \left[C_R m_{fu}, \frac{C'_R m_{ox}}{s} \right] \quad (1)$$

where m_{fu} and m_{ox} are the time averaged mass fractions of fuel and oxidant respectively; s denotes the stoichiometric oxygen to fuel mass ratio; $\min[]$ denotes the minimum of the

composition arguments; C_R and C''_R are empirically determined $O(1)$ constants. Together with a global, one step description of hydrocarbon combustion



only one reactive scalar requires computation, for example, the fuel mass fraction, m_f . The oxygen and product concentrations may then be determined from a statement of element conservation, represented by mixture fraction, for which one further scalar transport equation requires solution.

Energy conservation is represented by a transport equation for absolute enthalpy, defined as

$$\bar{h}_{mixture} \approx \sum_i \bar{Y}_i \bar{h}_i \approx \sum_i \left[\int_{T_{ref}}^T \bar{Y}_i C_{p_i}(\bar{T}) dT \right] + \bar{Y}_i h_{f,i}^o \quad (3)$$

where $h_{f,i}^o$, \bar{Y}_i are the enthalpy of formation and the mass fraction of species i . The sensible enthalpy is defined in terms of a specific heat as a function of the mean temperature.

One major concern in adopting the approximation implicit in Equation (1) is the omission of any dependence upon unmixedness and the high levels of scalar fluctuation, characteristic of turbulent burning. A second concern relates to the neglect of chemical reaction rates which vary dramatically with temperature through Arrhenius expressions.

Flamelet modelling provides a comparatively robust alternative to the eddy breakup model. Combustion is assumed to take place locally in the turbulent flame within microscopic elements which have the compositional structure of laminar flames. The latter take the form of state relationships for individual species as functions of mixture fraction, ξ .

$$m_i = m_i(\xi) \quad (4)$$

The state relationships may be derived from laminar flame measurement [1,9] or computation [10]. The flowfield prediction of Favre-averaged mixture fraction mean and variance, $\tilde{\xi}, \tilde{\xi}''^2$, permits a presumed shape *pdf*, $\tilde{P}(\xi)$, to be computed in standard form, typically via a Beta function.

$$\tilde{P}(\xi) = \frac{\xi^{\alpha-1} (1-\xi)^{\beta-1}}{\int_0^1 \xi^{\alpha-1} (1-\xi)^{\beta-1} d\xi} \quad (5)$$

where the parameters α and β are defined in terms of the mean mixture fraction and variance,

$$\alpha = \tilde{\xi} \left[\frac{\tilde{\xi} (1-\tilde{\xi})}{\tilde{\xi}''^2} - 1 \right] \quad (6)$$

$$\beta = (1 - \tilde{\xi}) \left[\tilde{\xi} (1 - \tilde{\xi}) / \xi'^2 - 1 \right]$$

The mean composition field may then be determined by quadrature from the state relationship, Equation (4)

$$\tilde{m}_i = \bar{\rho} \int_0^1 \frac{m_i(\xi)}{\rho(\xi)} \tilde{P}(\xi) d\xi \quad (7)$$

The above quadrature may be achieved by either a pseudo-analytical algorithm if the state relationships are expressed as simple polynomials or by numerical integration. It must be noted that integration of Equation (7) is required for each property represented by a flamelet description, at each grid node in the field model solution, at each iteration during the solution process. The quadrature process can therefore become computationally expensive. In the present study an accurate numerical integration scheme is employed prior to the field model solution to compute a lookup table of the integrand in terms of mean mixture fraction and variance. The lookup table represents a simple uniform discretisation of mixture fraction and variance space, typically on a 100x50 grid. Bi-linear interpolation is employed between discrete table values.

Radiation Heat Transfer

Thermal radiation is modelled using the discrete transfer radiation model (DTRM) [11]. The DTRM employs a ray tracing procedure whereby the radiative transfer equation (RTE) is solved along a finite number of ray paths determined by an *a priori* discretisation of the solid angle hemisphere normal to boundary cell faces. The change in radiative flux across an individual control volume is derived from the net balance between emission and absorption for all rays traversing that control volume. Summation of the final intensity at the end of a line of sight in all directions then yields the incident flux upon the boundary face. For grey boundaries the radiosity is represented by a combination of the emitted intensity and the reflected component of the incident intensity.

The transfer equation for thermal radiation along a ray in a direction \vec{s} may be written as,

$$\frac{dI}{d\vec{s}} = -(k_a + k_s)I + k_a \frac{E_g}{\pi} + \frac{k_s}{4\pi} \int_{4\pi} P(\Omega, \Omega') I(\Omega') d\Omega' \quad (8)$$

where, $E_g = \sigma T_g^4$ represents emission of radiant energy and $P(\Omega, \Omega')$ represents the probability that the incident radiation in the direction Ω' will be scattered into the increment of solid angle $d\Omega$ about Ω . The assumption is made that the soot is made up of small particles in this study, and so scattering is neglected. The formulation then reduces to,

$$\frac{dI}{d\vec{s}} = -k_a I + \frac{k_a \sigma T_g^4}{\pi} \quad (9)$$

Given a representative ray the intensity distribution can be calculated along it. This equation can be integrated to give the recurrence relationship,

$$I_{n+1} = \frac{\sigma T_g^4}{\pi} (1 - e^{-k_a \Delta s}) + I_n e^{-k_a \Delta s} \quad (10)$$

Thus the intensity may be calculated stepwise as the ray passes through successive control volumes within the domain. The initial intensity is calculated assuming that the surface is a grey, Lambert one,

$$I_0 = \frac{q_+}{\pi} = (1 - \varepsilon_w) \frac{q_-}{\pi} + \varepsilon_w \frac{\sigma T_w^4}{\pi} \quad (11)$$

Then at any given point on the boundary the incoming heat flux due to radiation is,

$$q_- = \int_{2\pi} I_w(\Omega) \cos \theta d\Omega \quad (12)$$

Clearly, q_- may only be calculated given knowledge of the initial intensity of the ray impinging on the surface of interest. Thus the process is iterative with updated initial ray intensities used at the beginning of each new iteration loop. The net wall radiative heat flux is simply the difference between the energy flux away from the surface and towards the surface.

Conventionally the discretisation of the solid angle in Equation 10 is achieved by equal division of polar and azimuthal angles. This choice leads to weightings proportional to $\sin 2\theta$ which produces a bias to rays closest to $\theta = \pi/4$. A detailed analysis has been performed [12] comparing results over a range of ray numbers where significant improvements in computational efficiency were demonstrated.

The optical properties of the combustion products were modelled using the Weighted Sum of Grey Gas approach, where the total emissivity is represented by

$$\varepsilon = \sum_j a_j(T) \left\{ 1 - \exp \left[-k_j (p_w + p_c) - k_j \rho_s f_v \right] \right\} \quad (13)$$

where p_w and p_c denote the partial pressures of H₂O and CO₂; ρ_s and f_v the soot density and volume fraction. The coefficients, a_j and k_j , are empirically determined, in the present study the coefficients of Truelove [13] were employed. It should be noted that more accurate, but time consuming, representations of the gaseous optical properties are available, these have been reviewed, in the context of a DTRM calculation by Bressloff et al [14,15].

Soot Formation

The principal contribution of this study is a generally applicable methodology for coupling between radiative heat transfer and the soot formation process within the framework of compartment fire prediction. The kinetic processes governing soot formation are commonly accepted to be nucleation, surface growth and coagulation, each of which is strongly dependent on temperature. Consequently the prediction of soot volume fraction is intimately coupled to the local radiative loss. The soot model employed [16,17,5] is based upon solution of transport equations for specific soot number density, ϕ_n , (normalised by Avogadro's

number) and soot mass fraction, ϕ_m , themselves directly related to soot number density, n , and soot volume fraction, f_v .

$$\phi_n = \frac{n}{\rho N_0} \quad : \quad \phi_m = \frac{\rho_s f_v}{\rho} \quad (14)$$

where ρ and ρ_s represent the gas mixture and soot density respectively.

The source terms in the respective transport equations are defined as [5]

$$\frac{d}{dt} \left[\frac{n}{N_A} \right] = \bar{\alpha} - \beta \bar{\rho}^2 \tilde{\phi}_m^{1/6} \tilde{\phi}_n^{11/6} \quad (15)$$

$$\frac{d\phi_m}{dt} = M_p \bar{\alpha} + \gamma \bar{\rho} \tilde{\phi}_n^{1/3} \tilde{\phi}_m^{2/3} - \omega \bar{\rho} \tilde{\phi}_n^{1/3} \tilde{\phi}_m^{2/3} \quad (16)$$

where α , β , γ , ω , are described by laminar flamelet state relationships; α accounts for the influence of nucleation on the number density and soot volume fraction; β , γ and ω characterise the processes of coagulation, surface growth and oxidation respectively. Each term is modelled in terms of properties describable by state relationships and empirical constants (pre-exponent and activation temperatures). These empirical constants are typically fuel type dependent [18], determined by comparison between prediction and experimental measurements in laminar flames. Consequently, mean values of the respective source terms are evaluated by integration over the local *pdf* of mixture fraction.

Non-adiabatic Flamelets

In general the mean value of a property (species concentration, temperature etc.) may be defined in terms of a joint probability distribution function over mixture fraction and enthalpy space (defined as enthalpy loss with respect to adiabatic).

$$\tilde{Y}_i = \int \int_0^1 Y_i(\xi, H_L) P(\xi, H_L) d\xi dH_L \quad (17)$$

In this study the unknown joint *pdf* is approximated by

$$P(\xi, H_L) \approx P(\xi)P(H_L) \quad (18)$$

where now the assumed Beta function *pdf* is employed within mixture fraction space and the *pdf* distribution for enthalpy is represented by a delta function centred upon the mean value of enthalpy. The net result of this simplification is that now mixture fraction state relationships for each property are required for each different value of mean enthalpy. The continuous enthalpy space is thus represented by a discrete number of points, for which an individual mixture fraction state relationship is required, between these points linear interpolation is employed.

A library of flamelets for enthalpy, temperature, species concentrations, soot source terms (etc.) are generated with each flamelet accounting for a different level of radiative loss. Then by comparison between the absolute enthalpy derived from solution of its transport equation with the statistically integrated values obtained from the flamelet library, it is possible to determine which temperature and density flamelets are required to evaluate the parameters in the soot model.

SIMULATION

Model Validation: Methane Burner

The coupled solution methodology is validated against experimental data obtained in a co-flowing turbulent methane jet flame [5]. In this case the flame is not buoyancy controlled and the associated turbulent length scales are constrained by the presence of the confining walls. Therefore the effect of turbulence/radiation interaction should be minimised in comparison to a pool fire within an enclosure and the configuration represents a test of the coupled soot and radiation modelling strategy.

Methane fuel is supplied via a 4 mm diameter orifice at a rate of 10.3g/min. The resulting jet flame is rim stabilised by an annular premixed pilot flame. The co-flowing air stream occupies the remainder of the inlet contained within a Pyrex cylindrical liner of 155mm internal diameter. The overall equivalence ratio is 0.25. Radial profiles of time averaged mixture fraction, temperature and soot volume fraction were made at flame heights of 150, 300, 350 and 425mm.

Predicted radial variations of temperature and soot volume fraction are compared against the experimental data at heights of 150, 300 and 425 mm in Figures 1 and 2 respectively. Agreement between the coupled soot and radiation predictions and the experimental data are reasonable. Centre line temperatures and soot volume fractions are well predicted though the radial distribution is less well represented, this may be partly attributed to known deficiencies in the k- ϵ turbulence model when predicting axi-symmetric jets. Also shown for comparison are results from an uncoupled calculation where radiation was not accounted for - not surprisingly the predicted gas temperature is higher, resulting in much greater soot formation rates. This simple example illustrates the necessity for a coupled soot and radiation calculation if any form of detailed reaction kinetics are to be incorporated.

Model Demonstration : 600 kW Room Fire

Whilst there are significant differences between the laboratory scale flames typically employed in model development and practical fires, the preceding comparisons demonstrate that the methodology for coupling radiation heat transfer and soot chemistry does introduce the necessary physical realism and is computationally tractable. Detailed spatially resolved property measurements are not presently available for compartment fires, but we here provide a demonstration of the application of the same approach to field model simulation of an illustrative room fire.

Consistent with the jet flame predictions, the fire source is a methane-fuelled burner of square cross-section and the enhanced levels of soot which are computed simply reflect the increased scales and residence times typical of such fires. The ceiling layer development, now characterised by smoke concentration, figure 4, is similar to that observed in earlier,

over-ventilated, Steckler-type room fire simulations, using other scalar markers (cf. Lewis et al [6], and the computed soot concentration profiles mimic those of temperature quite closely (cf. figs 2,3). At the modest temperature levels observed in the ceiling layer with 600 kW heat input, soot production and oxidation are restricted to the buoyantly-driven plume and the soot levels elsewhere in the compartment are established principally by turbulent mixing and dilution (figs. 5,6).

Extension of the strategy to different , more heavily sooting fuels in order to explore, for example, the prediction of radiation induced flame spread and quantitative smoke transport (and hence obscuration) requires that the data-base on non-adiabatic flamelet state relationships be substantially enlarged. Such developments are presently underway at Cranfield.

CONCLUSIONS

A laminar flamelet-based strategy for the coupled field model prediction of smoke production and radiation heat transfer in fires has been developed and demonstrated in a laboratory scale turbulent flame, in which the combustion source has been experimentally mapped in finely-resolved detail, and then in a representative compartment fire. The influence of radiative loss on the temperature dependent sooting processes, and hence the requirement to model their interaction, is clearly illustrated.

The approach adopted can be readily extended to other fuel sources for which laminar flamelet data can be made available from experimental measurement or from detailed laminar flame computation. An important extension to existing field modelling is then introduced by the coupled prediction of radiative heat fluxes to neighbouring surfaces, since this permits the simulation of time-dependent fire growth in compartments which also embrace surface flame spread mechanisms.

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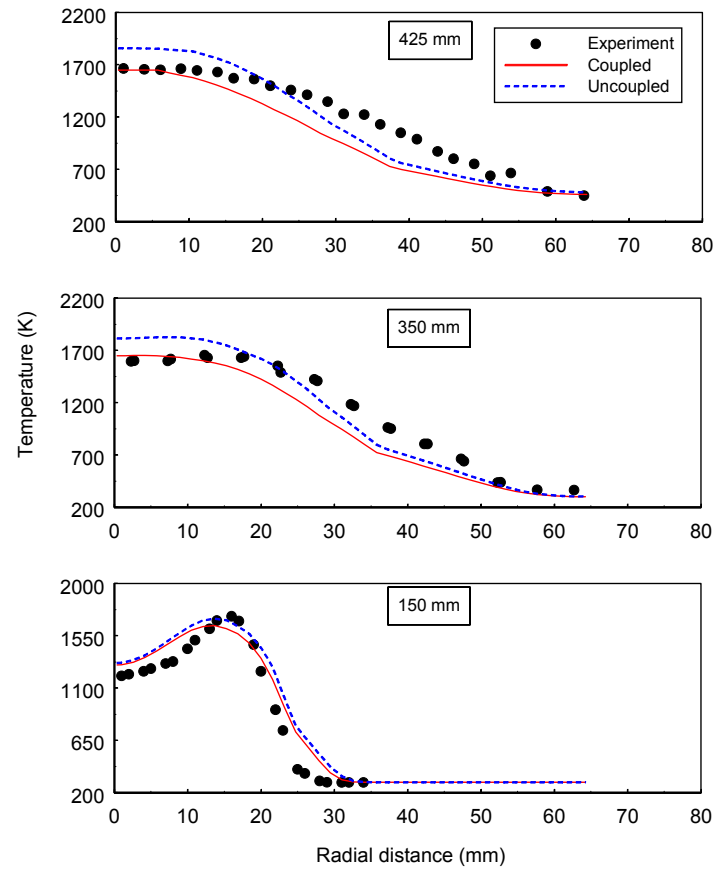


Figure 1: Methane Jet Flame - Radial temperature profiles
Coupled - with coupled soot and radiation model;
Uncoupled - No radiation.

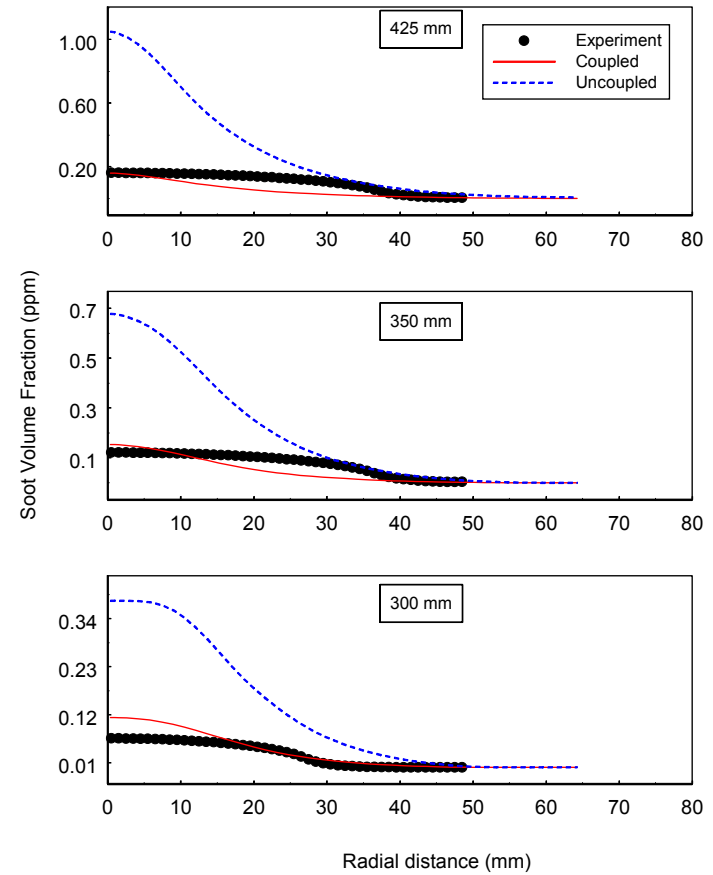


Figure 2: Methane Jet Flame - Radial soot volume fraction profiles
Coupled - with coupled soot and radiation model;
Uncoupled - No radiation.

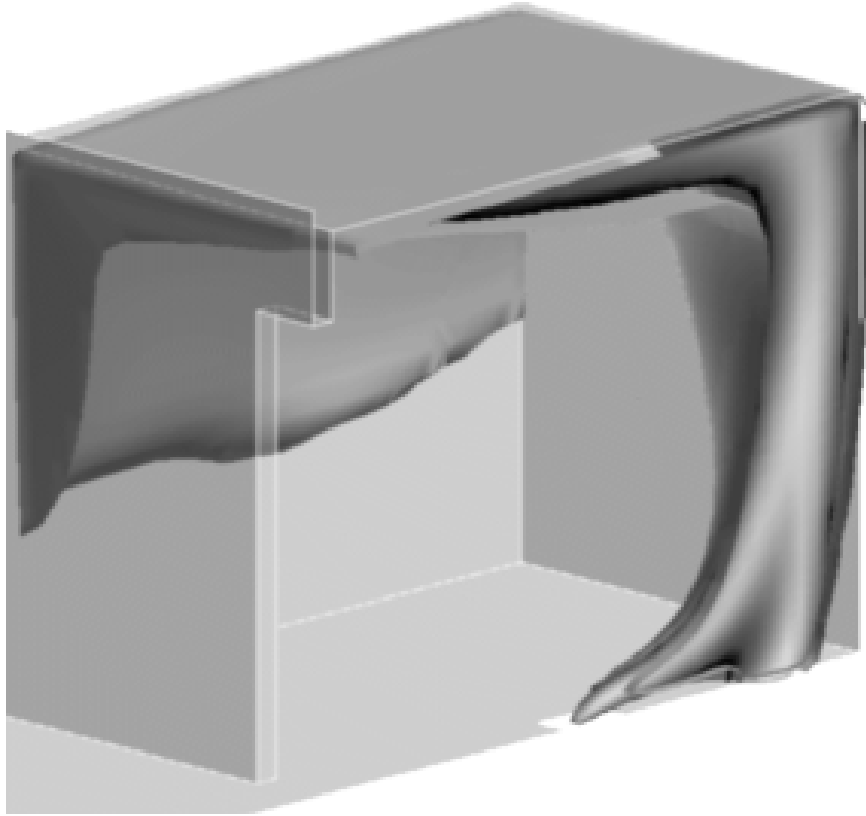


Figure 3: Visualisation of pool fire illustrating half of compartment with soot volume fraction isosurface at 0.5ppm

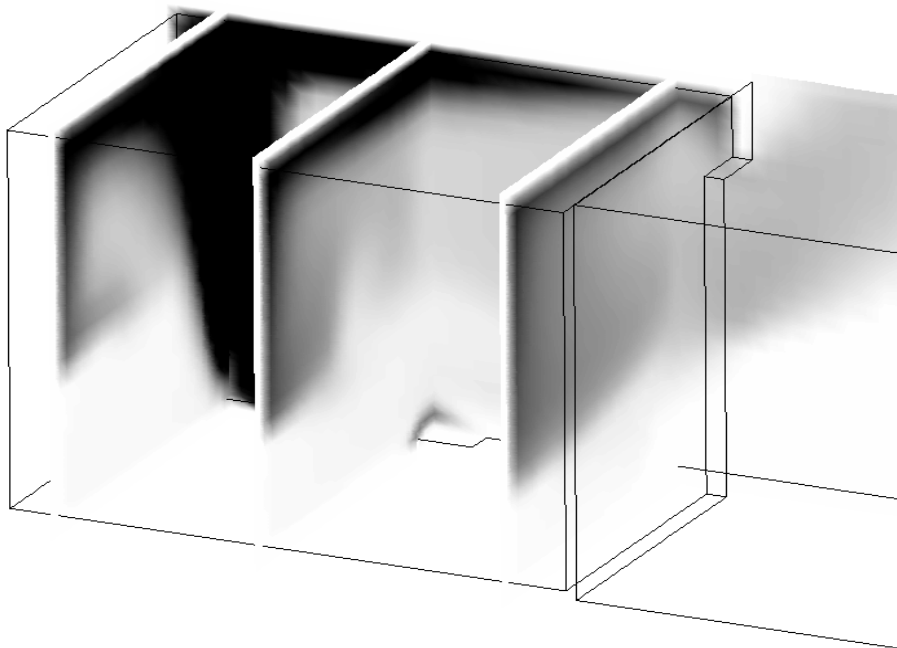


Figure 4: Visualisation of smoke layer within compartment

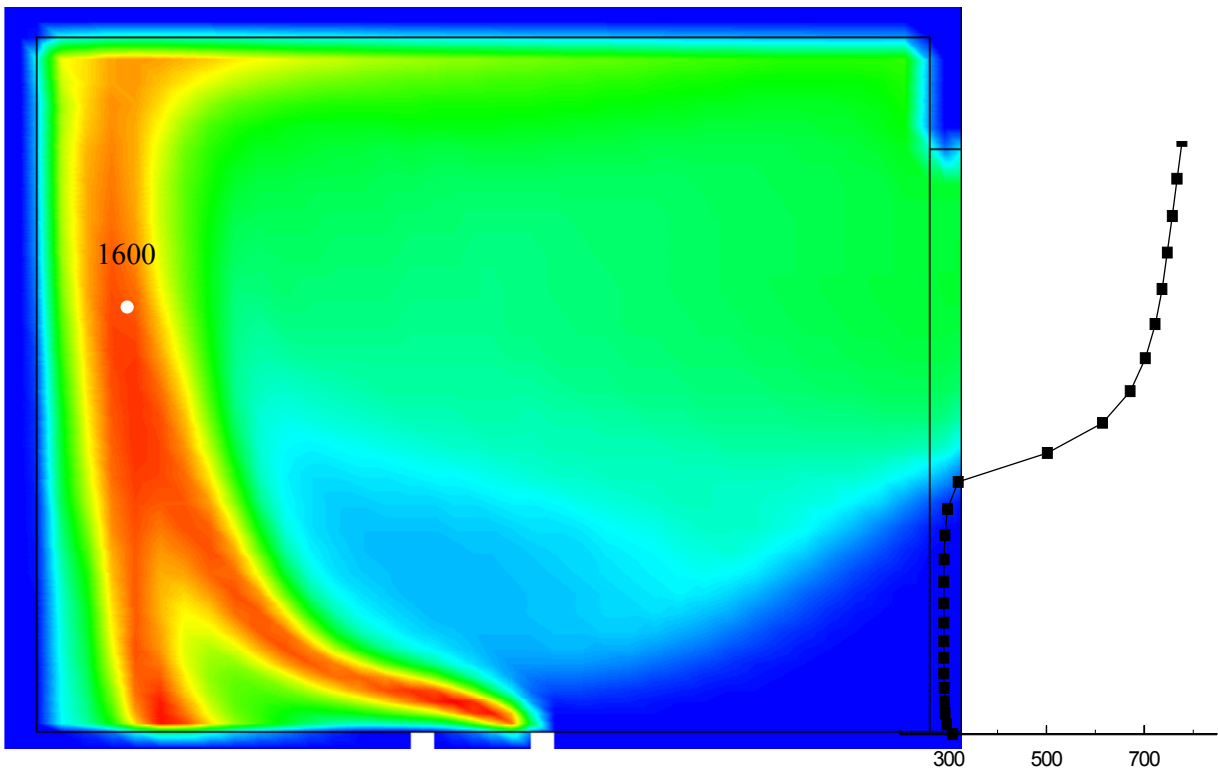


Figure 5: Predicted gas temperature on room centre line and vertical profile through doorway (K).

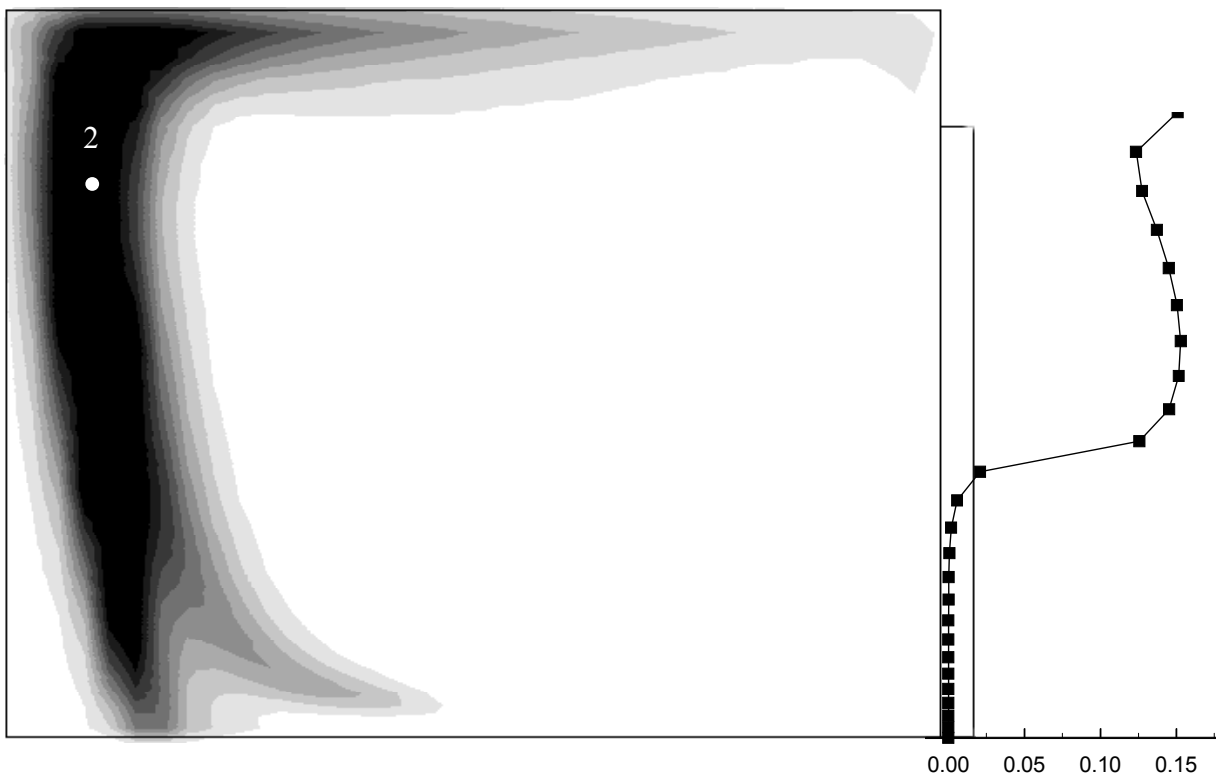


Figure 6: Predicted soot volume fraction on room centre line and vertical profile through doorway (ppm)