

Modelling CO Production in Vitiated Compartment Fires

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ABSTRACT

Strategies for the modelling of CO production in compartment fires, based on laminar flamelet relationships, derived from computations of vitiated laminar diffusion flames, and on a simplified two-step eddy dissipation model, are identified and compared. A flamelet library is constructed which incorporates the parametric variation of ambient oxygen concentration and temperature. Expected departures from mixing controlled burning, arising in regions like hot ceiling layers, for example, are assessed with reference to homogeneous plug flow calculations, initiated from peak CO conditions drawn from the laminar flame computations. Implementation of the two approaches in CFD simulations of ventilation-controlled compartment fires using the SOFIE code suggest that both offer the prospect of reliable CO prediction, given a measure of calibration.

KEY WORDS: carbon monoxide, compartment fires, field modelling

INTRODUCTION

Products of incomplete combustion - carbon monoxide and smoke - represent the principal life threat in most building fires. Whilst CFD based simulation of fire plume development is now an established feature of much fire safety assessment for public buildings, most attention has focussed on 'smoke' movement as reflected in the passive transport of a scalar marker - typically a modest temperature isotherm or lower bound mixture fraction. Detailed concentration predictions have not been incorporated into these analyses. Once all chemical reaction has been effectively quenched, as a result of product dilution and heat loss to boundaries, the characterisation of the hazard in terms of non-reactive scalar mixing would appear entirely appropriate. The difficulty in making this approach quantitative clearly lies in establishing the implied near-frozen CO concentrations emerging from the fire source. Under ventilation-controlled conditions the fuel-rich plume in a typical compartment fire extends into the ceiling layer and is accompanied by continued burning under increasingly vitiated conditions. The customarily employed single-step, mixed-is-burnt description of the combustion process is ill-suited to the modelling of processes such as these in which finite rate chemistry plays a significant role. This paper describes the application of laminar flamelet modelling to the problem and seeks to assess, through further detailed kinetic modelling, the range of conditions over which this approach can be considered appropriate. The methodology employs a flamelet library in which the extent of ambient vitiation - as represented by the uncoupled variation of temperature and gas composition with mixture

fraction - is included. Comparisons are also reported with predictions based on a simpler two-step eddy break up representation of the combustion process in which global CO production is identified explicitly.

One of the more distinctive features of naturally ventilated compartment fires is that the fire source is often remote from the air inlet, which may also act as the exhaust for combustion products. Mixed flow ventilation of this type promotes vitiation of the ambient air with partially-cooled CO₂ and H₂O. The mixture fraction alone cannot characterise this behaviour and the customary flamelet relationships must address both the reduced oxygen content and the heat loss, at least in parametric form.

The inclusion of complex, finite rate chemistry in the practical simulation of combustion problems always raises concerns for the compromise between ease of application (robustness, resource level, turn-around) and quality of prediction. The situation in relation to fire is further complicated by the large extent of the typical solution domain which constrains the resolution possible. As a result, the fire research community has to date been slow to explore the more computationally intensive options – for example, pdf transport methods or conditional moment closures. In this environment considerable advantages accrue to flamelet models over those more detailed approaches which address the direct integration of multi-step rate processes, provided the underlying approximations can be demonstrated to be robust.

In its simplest interpretation the localised burning zones in the fire, where the principal chemical activity is concentrated, are considered to be similar to those of a steady-state laminar diffusion flame, burning under the same conditions. This microscopic flame structure, free from the uncertainties introduced by turbulent fluctuations and buoyancy in the fire, can be computed exactly within the limits of our understanding of the detailed chemical kinetics. In his detailed review of the processes giving rise to CO production in fires, Pitts [1] identifies several important mechanisms which do not readily admit of a flamelet interpretation, however. One such is the situation in which the burning plume penetrates into a hot, oxygen-deficient ceiling layer. Continued chemical reaction is to be expected in this near-homogeneous layer, albeit slow, and the associated scalar structure is perhaps poorly represented by that of the fuel-rich wings of a laminar diffusion flame. The extent of likely departures from more nearly mixing-controlled combustion will therefore be evaluated here too.

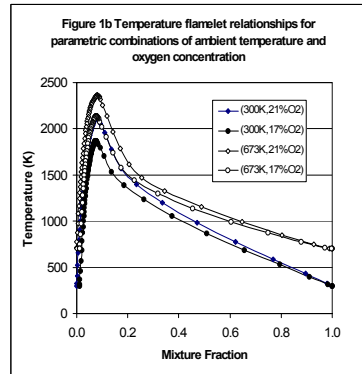
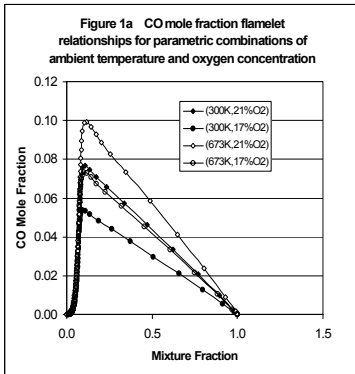
LAMINAR FLAME COMPUTATION

A range of numerical simulations has been performed for laminar diffusion flames in a conventional counter-flow configuration under freestream boundary conditions of varying oxygen concentration and temperature. The steady-state calculations have been performed within a code first developed by Warnatz and co-workers [2] and incorporate a detailed reaction mechanism drawn from the CHEMKIN kinetics database [3].

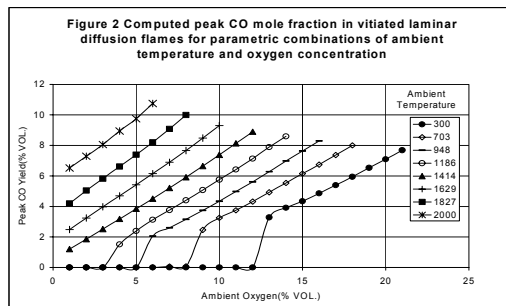
The flames investigated are fuelled by ethylene. The soot-free kinetic mechanism is comparatively well-established - here incorporating 53 chemical species and 296 reaction steps - and the fuel carbon-hydrogen ratio is representative of a broader range of

practically relevant combustible materials. The freestream oxygen concentration is varied from that of standard air down to levels, vitiated with stoichiometric combustion products (CO_2 , H_2O and N_2), which will not sustain combustion. The freestream temperature is varied independently of the vitiation level in order to accommodate the effects of variable heat loss to the surroundings in the compartment fire.

Figure 1 illustrates the variation of CO concentration and temperature with mixture fraction, in flames for which the ambient O_2 concentration is reduced from 21% to 17%, whilst the accompanying temperature is increased from 300 K to 673 K. Although, as expected, both the peak CO concentration and temperature are highest under conditions in which standard air (21% O_2) is effectively pre-heated to 400°C , the reaction zone temperature distributions for standard air at 300K and for 17% O_2 at 400°C are broadly comparable and generate very similar peak CO at approximately 7.5% by volume.



The combined effects of heat loss from combustion products, by convection or radiation heat transfer to the compartment walls, and reduced oxygen level can evidently exert a significant influence on the CO produced in the fire source.



A comprehensive summary of the simulations is provided by Fig 2 in which the peak CO yield from a wide range of simulations is plotted against the ambient oxygen level at progressively increasing initial temperatures. Each curve has an upper bound corresponding to vitiation by adiabatically-heated combustion products. As the ambient temperature is increased, the limiting oxygen concentration for stable burning falls. By

way of illustration, we note that at an ambient temperature of 300K the peak CO concentration falls steadily with the level of vitiation (by cooled combustion products) until the O₂ concentration reaches 12% by volume at which point the flame is extinguished. If the initial temperature is increased, the peak CO level is raised and the flammable range is extended down to ever greater levels of vitiation - down to $\leq 5\%$ at 1200K. The increases in peak CO concentration are quite modest, however, and do not approach the levels in excess of 20% that might be expected under conditions of complete chemical equilibrium. The flame structure here is everywhere determined by the balance between mass diffusion and rates of chemical reaction, and not by equilibrium thermodynamics.

These calculations can be used to establish a flamelet library in which the state relationship between a particular flame property, ϕ_{α} , and the mixture fraction, ξ , is defined for parametrically varying freestream conditions of vitiation (O₂ level) and temperature. For example, in respect of the CO concentration

$$X_{CO} = X_{CO}(\xi ; T_{ambient}, X_{O_2, ambient}) \quad (1)$$

Under the assumption that CO production, wherever it occurs in the turbulent fire plume, arises from flamelet-like, thin flame burning, then knowledge of the local mixture fraction is sufficient to define the complete burning state through Eq.1. In other flamelet modelling applications these state relationships might also be characterised by the hydrodynamic strain rate, but the freely burning fire is a relatively benign strain environment in comparison with most practical combustion systems and therefore such influences may be neglected. The nominal strain rate employed in calculations here is 100s⁻¹.

COMPARTMENT FIRE SIMULATION

Laminar flamelet modelling

The vitiated laminar flames computed in the previous section have been incorporated into the field modelling code SOFIE [4] for purposes of compartment fire simulation. SOFIE is a general three-dimensional curvilinear code, developed at Cranfield specifically for the simulation of fires in enclosures. It employs finite volume discretisation and a range of options for interpolation (Upwind, Hybrid (employed in the computations reported here), QUICK and TVD), together with the SIMPLEC pressure correction algorithm applied to co-located velocities and pressure. In the flamelet approach to combustion modelling, balance equations for the mean and variance of mixture fraction are solved in addition to those for momentum, continuity and the turbulence properties, k and ϵ , from which the eddy viscosity coefficient in the Boussinesq approximation is calculated. The turbulent kinetic energy equation incorporates the standard correction for buoyant production.

Although the peak levels of soot volume fraction may be a little lower in vitiated flames than in their unvitiated counterparts, radiative exchange will clearly be a factor in all these flames. The coupled prediction of soot production and thermal radiation, even for

simpler gaseous fuels, remains a challenging problem, however, and some uncertainty surrounds the treatment of burn-out when a single conserved scalar is used to characterise the multi-dimensional scalar field involving turbulent mixing and chemical reaction [5]. The processes of soot formation and oxidation are comparatively slow and therefore soot volume fraction cannot be accommodated in an explicit flamelet relationship of the type in Eq.1. Additional balance equations must therefore be solved for at least two soot scalars, typically soot volume fraction and number density. In the present study, however, in order to limit the complexity of the modelling introduced for the chemical composition and thereby focus specifically on CO production, the multiple flamelet soot model available in SOFIE [6] has been omitted in favour of a simpler alternative. Specifically, the effect of radiative loss is accommodated by introducing a single fixed enthalpy loss into the vitiated temperature flamelet relationships such that

$$T = T(\xi; X_{O_2, ambient}, T_{ambient}, \chi_R = 0.25) \quad (2)$$

where χ_R denotes the prescribed level of heat loss, here set to 25%, which is distributed uniformly as a fraction of the sensible enthalpy.

The influence of turbulent fluctuations within the fire source on the mean property prediction is accommodated through the probability density function for mixture fraction $\tilde{P}(\xi)$, determined from the computed values of the mean and variance of mixture fraction, whence, for example,

$$\bar{T} = \bar{\rho} \int_0^1 \frac{T(\xi; X_{O_2, ambient}, T_{ambient}, \chi_R = 0.25)}{\rho} \tilde{P}(\xi) d\xi \quad (3)$$

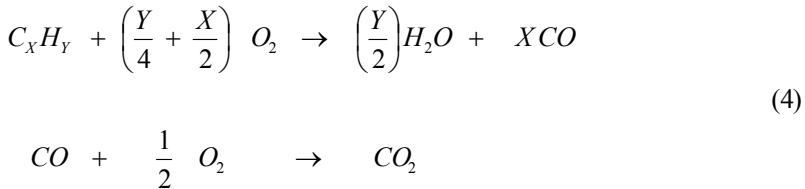
Given this underlying framework, the critical step in the implementation of the vitiated flamelet relationships in the simulation is the selection of the appropriate level of vitiation, as represented by the ambient oxygen concentration and temperature. The most direct approach is simply to select a region within the computational domain to act as a marker for the vitiated ambient, from which an average level can be determined. Some knowledge of the flowfield and, in particular, the pattern of ventilation is evidently necessary to establish this, but preliminary computation could supply this information if inspection alone is insufficient. In transient simulations a strategy of progressive changes to the vitiation level can be similarly adopted.

Two-step eddy break-up formulation

The majority of fire simulations continue to employ variants of the eddy break-up or eddy dissipation concept [7]. Whilst the shortcomings of this representation have been well documented (for example, [8]), the model is simple to apply and robust in practical

application. It serves to distribute the heat release in a realistic manner and therefore couples the fire plume to the buoyancy dominated flow in a generally satisfactory fashion. It also tends to over-predict gas temperatures, however, because the influence of turbulent scalar fluctuations is poorly represented and the description of the combustion product state is usually restricted to the major stable species, CO₂ and H₂O, alone. The formulation can be extended to incorporate two semi-global steps, however, admitting the computation of CO.

In its simplest form, the model considers the rate limiting process in non-premixed combustion to be that of small-scale turbulent mixing between the reactants. This proceeds at a rate determined by the turbulent kinetic energy, k , and its rate of dissipation, ε . Specifically, we can introduce a simplified mechanism for hydrocarbon combustion of the form



where the rate limiting mass consumption rate for reactant may be that of the hydrocarbon fuel or of the oxygen. CO production is then determined by

$$R_{CO,prod} = \phi_{CO} [\rho Y_{C_xH_y} (\varepsilon/k), \kappa \rho Y_{O_2} (\varepsilon/k) / S_1]_{\min} \quad (4a)$$

where ϕ_{CO} denotes the mass of CO produced per unit mass of fuel consumed in reaction (1), κ is an empirical constant and S_1 denotes the stoichiometric mass ratio of oxygen to fuel. CO consumption is similarly determined from

$$R_{CO,con} = - [\kappa' \rho Y_{CO} (\varepsilon/k), \kappa'' \rho Y_{O_2} (\varepsilon/k) / S_2]_{\min} \quad (4b)$$

where S_2 denotes the stoichiometric ratio for reaction (2) and κ', κ'' are again empirical constants.

The chemical source term in the balance equation for CO mass fraction is then the sum of these two terms.

RESULTS AND DISCUSSION

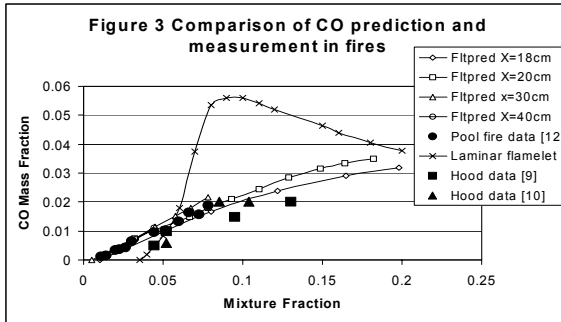
Combustion modelling

Many analyses of CO production in compartment fires have been constructed within the framework of zone modelling which encourages the development of experimental

analogues for widely observed fire features. The burning fire plume penetrating the ceiling layer is one such feature and this has been represented at laboratory scale by fires burning under ventilation-controlled hoods [9,10]. Characterisation of conditions under the hood in terms of equivalence ratio has then provided a basis for CO correlation, subject to some caveats regarding the extent and nature of the process by which ambient air is entrained into the plume [1]. Since the local mixture fraction, ξ – the scalar variable central to the fast-chemistry, mixing-controlled combustion models employed in the field modelling of non-premixed flames [11] – is related to the local equivalence ratio, ϕ , quite simply,

$$\xi = (1 + AFR)^{-1} = (1 + [AFR]_{stoich} \phi^{-1})^{-1} \quad (5)$$

it is instructive to compare flamelet-based CO predictions with measurements in both open fires and the hood experiments under-pinning the Global Equivalence Ratio (GER) concept [1]. Figure 3 presents a comparison between measurements in methane fuelled fires and numerical predictions based on laminar flamelet modelling. The measurements comprise data from within the flaming region (27cm height) of laboratory-scale, burner-simulated pool fires at heat release rates of 18 and 47kW [12] and those from widely reported hood experiments [9,10]. The numerical predictions are taken from the early study of methane pool fires reported by Crauford et al [13] at different axial positions in a similarly sized fire.



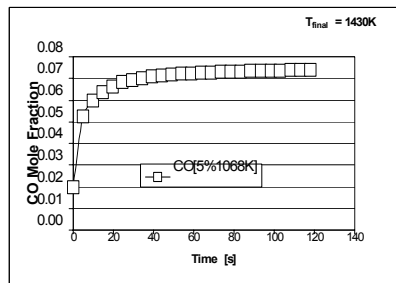
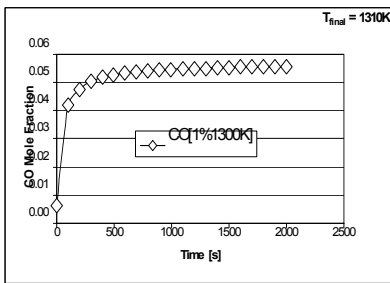
For reference purposes, the CO flamelet state relationship underlying such modelling is also shown. It must be recognised, however, that this latter relationship describes the ‘exact’ instantaneous state relationship, whilst all the other properties from the fire are time-averaged and involve integrals of state properties over the probability density function for mixture fraction. It appears that within typical levels of experimental uncertainty for probe sampling measurements in turbulent environments, there is little difference between the sets of CO yield data. Similar levels are produced, whether in a freely-burning - and overall, over-ventilated - fire or under a hood, and furthermore that flamelet-based modelling provides a plausible representation of CO production in such circumstances. Both experiments were performed at relatively small scale, however, and whether conditions that more nearly approach those of chemical equilibrium might prevail in large fires is unresolved.

In order to inform this discussion a series of homogeneous reactor computations have been performed, starting from conditions that would appear representative of fire plumes.

The calculations have been performed using the *Plug* routine within the CHEMKIN program suite [3]. The reaction mechanism adopted is the widely used *GRI Mech* for hydrocarbon combustion [14]. The simulations envisage that the flame plume is quenched upon entering the upper layer but further reaction continues in a substantially homogeneous manner, without additional air entrainment. Figure 4 compares the time evolution of the CO concentration, from compositional starting conditions derived from the opposed diffusion flame calculations reported earlier. The underlying laminar flame relationships, selected here for display, incorporate varying levels of both ambient vitiation and temperature but lead to broadly comparable temperatures in the presumed homogeneous layer, specifically, in the range 1310 K -1500 K. Though arbitrarily chosen, such values are considered representative of ceiling layers where heat loss to the walls limits the maximum temperatures attained. The initial conditions for the plug flow calculation are taken to be those accompanying the peak CO concentration for the particular laminar flame. Under conditions typically promoting further CO generation in the upper layer - corresponding to the least ambient vitiation - the CO concentration rises from an initial level of approximately 4% to in excess of 8%, but over a timescale approaching 1 minute. The final levels are observed to decrease, however, and the necessary residence times increase, with the level of vitiation initially.

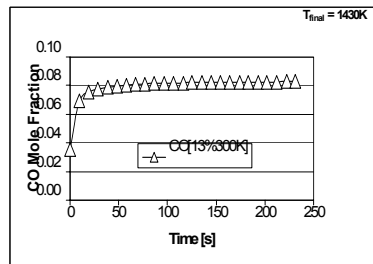
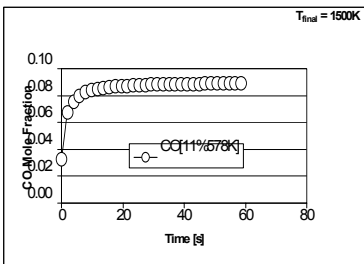
Figure 4 Plug Flow calculations of CO evolution

- (a) Initial state: flamelet peak CO for 1% O₂ and 1300K ambient (b) flamelet peak CO for 5% O₂ and for 1% O₂ and 1068K ambient



- (c) flamelet peak CO for 11% O₂ and 578K ambient

- (d) flamelet peak CO for 13% O₂ and 300K ambient

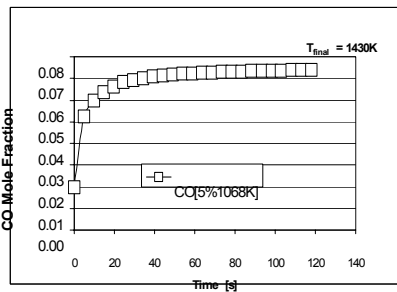
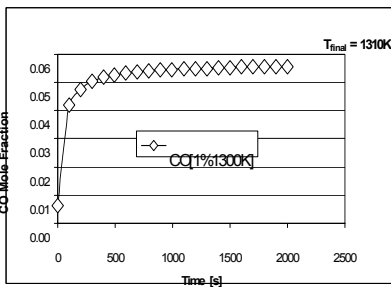


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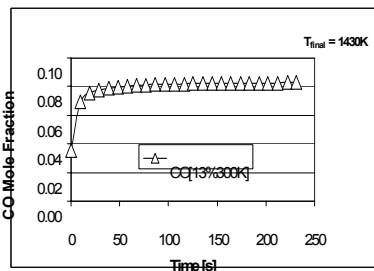
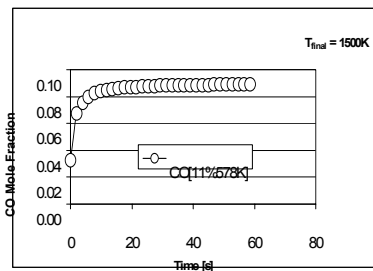


Figure 5a Distribution of mean temperature ; 1 MW compartment fire, 2-step eddy dissipation model

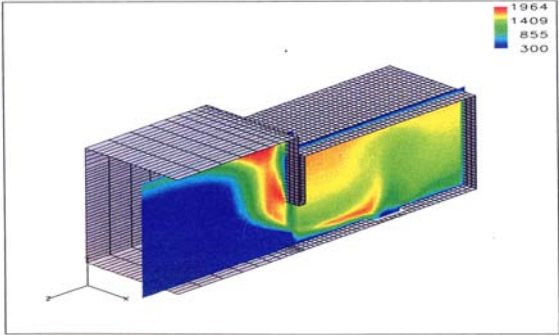


Figure 5b Distribution of CO mole fraction; 1 MW compartment fire, 2-step eddy dissipation model

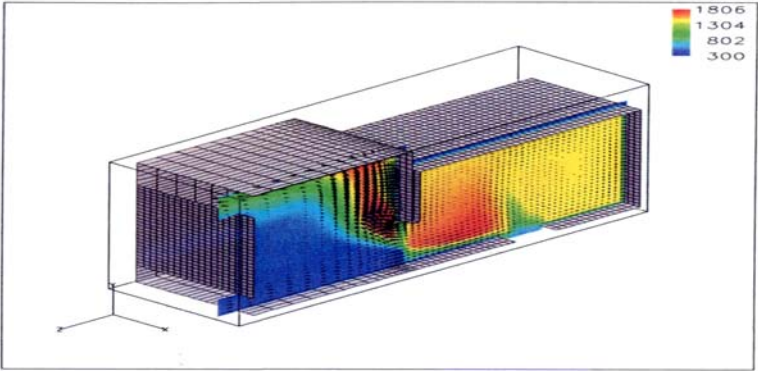


Figure 6a Distribution of mean temperature; 1MW compartment fire, laminar flamelet model [17%O₂ and 473 K]

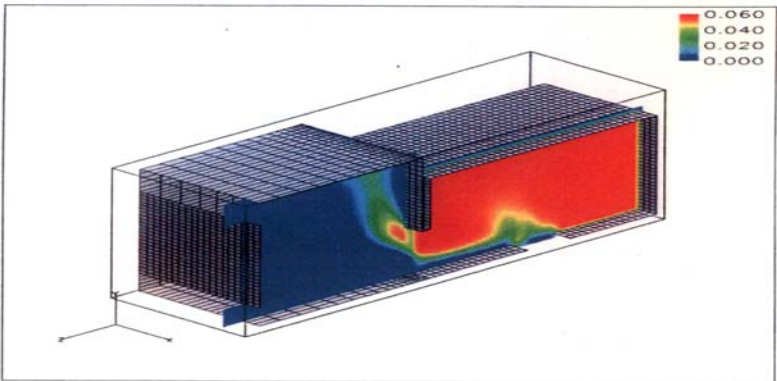
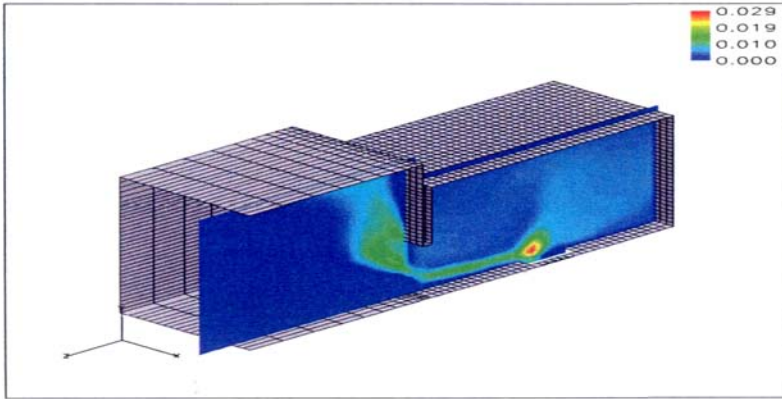


Figure 6b Distribution of CO mole fraction; 1 MW compartment fire, laminar flamelet model [17%CO and 473K]



Both models require some measure of calibration. The coefficients in the EBU expressions (κ , κ' , κ'' in eqns.(4a,b)) were taken from the simulations of vitiated jet flames reported by Hyde and Moss [17] and may be inappropriate to the under-ventilated compartment fire. On the other hand, the choice of vitiated flamelet relationship (17% O_2 , 473 K) is arbitrary and could be subject to more detailed sensitivity analysis, given the computed conditions in the compartment doorway. Both models do hold out the promise of realistic CO prediction, however, and encourage more extensive comparison with spatially-resolved measurement in under-ventilated compartment fires.

CONCLUSIONS

The paper describes the development of two models for CO production in fires, based on detailed laminar flamelet state relationships embodying different levels of ambient vitiation and on a simpler two-step eddy dissipation formulation. For a broadly representative hydrocarbon fuel - ethylene - the laminar flame computations indicate that peak CO will not exceed 10%. If heat loss and turbulent fluctuations are then taken into account, CO levels from homogeneous phase processes in fires are unlikely to exceed 5-6%. Plug flow calculations suggest that further reaction in partially-cooled ceiling layers will not substantially increase these values and they will remain well-below the values inferred from rich equilibrium computations. Both models have been implemented in the Cranfield SOFIE code and applied to an under-ventilated compartment fire. Though the results are encouraging, further detailed comparison with experiment is necessary to discriminate between the approaches and to provide the necessary calibration under conditions removed from those readily available from laboratory experiment.

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