PREDICTION OF TOXIC SPECIES IN FIRE

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INTRODUCTION

Recent years have seen renewed interest in developing and exploiting methods for prediction of toxic species in fire. Whilst fire modelling, specifically the techniques of computational fluid dynamics (CFD), has seen increasing use for fire safety engineering analysis, e.g. for design of smoke control systems, attempts at the quantitative evaluation of toxic species have hitherto been confined to research environments. The reasons for this are well known – the challenge of adequately describing the combustion chemistry in real fires, typically involving multiple, complex, and uncertain fuel sources, with underventilated burning often dominating, far exceeds the demands of predicting just the *transport* of combustion gases. And we often do not even know the required inputs, i.e. the kinetics of the solid-phase pyrolysis or the gas-phase reactions of the liberated volatiles.

Toxic species emissions are nevertheless of great interest, considering their often significant impact on life safety. Thus there are a number of avenues of potential exploitation, including fire forensics, in supplementing standard testing and ultimately in use for design. The availability of modelling tools which provide the option of simulating carbon monoxide (CO) generation is also pushing forward the demand for improved predictive capabilities, as users seek to verify, validate and apply the latest models. This paper overviews the state of the art in this field, highlighting current research with Computational Fluid Dynamics (CFD) models and some of the remaining limitations and deficiencies which provide a constraint on the wider application of these simulation tools.

TOXIC SPECIES IN FIRE

In order to appreciate the modelling challenge it is useful to consider the range of phenomena we hope models will ultimately be able to capture. The broader definition “toxic species” would include all products of combustion that are harmful to health, encompassing asphyxiant and irritant gases. The range of species of interest and their impacts on human subjects are comprehensively described in various chapters of the recent text, “Fire toxicity”, eds. Anna Stec & Richard Hull (2010). Though there may be some debate about the role played by individual components in cases of fire fatalities, it is generally recognised that carbon monoxide is the most significant asphyxiant and often the main cause of incapacitation and ultimately death (Purser 2010a); in the presence of nitrogen containing materials hydrogen cyanide may also be an important factor in incapacitation, but it will invariably be associated with high levels of carbon monoxide, acting additively. Likewise, smoke and irritant gases will in practice have an important role in fatalities simply by impairing escape activities (Purser 2010b). Irritants compositions are more directly associated with the chemical composition of the burning materials. Descriptions of the combined effects of hazardous species (and heat) are provided in fractional effective dose (FED) models (Purser 2010c). Whilst these methods provide a means of estimating the cumulative impact given any set of fire conditions, in practice the typically dominant role of carbon monoxide, and uncertainties in other species, means that it is often taken to be representative of the entire "toxic species" problem. Here we confine our attention to CO alone, whilst recognising this assumption.

Formation mechanisms

A significant amount of research has been undertaken towards understanding the fundamental pathways of CO production in fires. Pitts (1995) provided a comprehensive review identifying distinct mechanisms resulting in CO yields. Earlier work had focused mainly upon the value of correlating CO to a Global Equivalence Ratio (GER, or φ) parameter representative of the averaged species compositions with the fire zone, this being equal to unity for stoichiometric combustion, and CO levels typically rising rapidly under underventilated combustion conditions associated with values greater than one. Pitts isolates three further mechanisms, associated with the continued mixing of air into rich upper layers, the liberation via solid-phase pyrolysis with cellulosic combustibles, and approach to equilibrium at high temperature. Each mechanism gives rise to more CO, thus the GER model can only provide a non-conservative lower limit on yield for certain restricted conditions, which unfortunately do not extend to the practical fire scenarios of most concern from a life safety perspective, i.e. remote transport of combustion products from under-ventilated post flashover fires. This defines the challenge for more comprehensive and realistic models (Paul & Welch 2010).

Some further details are worth noting. Though initial studies demonstrated that the GER parameter was capable of collapsing CO yields, in a manner essentially independent of the burner size and upper layer temperature in the range 470-800K (Beyler 1983), further work found a measurable impact of upper layer temperature (Morehart 1990). Given that fuel dependences were also known, with evidence of rough groupings by fuel structure for both hydrocarbons (Beyler 1983) and solid fuels (Beyler 1986) there was still hope that correlation based approaches may prove sufficient to "predict" CO concentrations for simple fuels and well-defined upper layer temperatures. However, the other mechanisms identified by Pitts undermined the idea of unique correlations. Measurements in reduced scale enclosures indicated that direct air entrainment into hot fuel-rich upper layers was giving rise to generation of more CO. With continued reaction in the layer residence time effects also become important, i.e. we are dealing with finite-rate chemistry in which the resultant yields depend on the thermodynamic histories of each element of fluid. CO yields were found to be approximately doubled in full-scale enclosures, this also being attributed to differences in upper layer temperatures. When upper layer temperatures approaches 1400-1500K kinetic studies confirmed that approach to equilibrium concentrations (~16% at φ=3). Finally there are the observed effects of liberation of CO via the pyrolysis of cellulosic materials, for example in fires involving fuels or compartment linings made out of wood. The net result is very high yields of CO even in reduced scale, exceeding 10% volumetric concentrations (Pitts 1995).

Thus we have a number of essential mechanisms or CO production which for general cases of interest, e.g. under-ventilated post-flashover environments, do not permit simple correlation of liberated CO yields to any instantaneous underlying thermodynamic parameter. These phenomena clearly define the requirements for any true predictive capabilities, making clear that explicit treatments of finite-rate chemistry will be required, together with solid-phase models where these are relevant to the scenarios being modelled. The challenge of representing these behaviours within the frameworks of tractable computational models is outlined next.

MODELLING APPROACHES

In recent years, many numerical studies of CO formation in fires have been conducted, see review by Welch *et al.* (2010) for more details. An assumption is made that CFD-based models are of prime interest, these being the only approach with a comprehensive basis permitting coupling of the essential phenomena at a fundamental level. Amongst CFD models applied to representation of toxic species a range of diverse approaches have been adopted, each with different strengths and weaknesses associated with factors to do with generality versus empirical dependence, uncertainty in required inputs and computational demands. Here we discuss some of the more promising approaches, focussing on those at the lower end of complexity and computational requirements, i.e. likely to be most practical in the hands of practitioners.

A class of combustion model known as the laminar flamelet approach has found wide application in reactive flow problems and provides a consistent description of heat release and detailed reaction chemistry. Its main attraction is the fact that it works on assumption of correlation to a conserved scalar parameter, i.e. the mixture fraction, this representing fuel-derived mass with the reacting flow – conserved because it can neither be created nor destroyed, purely transported around the domain, via processes of convection and diffusion. Thus by solving just two transport equations, for mixture fraction and its variance, it is possible to “lookup” the chemical composition of any portion of mixture, determining it uniquely. This composition can be obtained from detailed kinetic calculations, which may be of arbitrary complexity because they are performed off-line, i.e. prior to running the fire simulation. In case of uncertain kinetics, or otherwise, direct results of experimental investigations can be invoked to establish the mixture fraction correlations, i.e. flamelet lookup value. However, as per the discussion of the previous section the problem at hand may often require explicit treatments of finite-rate chemistry. The traditional flamelet approach, i.e. steady laminar flamelet models (SLFM), does allow for the reaction-flow interaction, thus a partial relaxation of the fast chemistry assumption of simpler combustion models such as eddy break-up. It might even be parameterised in terms of strain rate, and other relevant parameters such as heat loss (Young & Moss 1995) or vitiation (Tuovinen & Simonson 2001), but it remains essentially an instantaneous representation with no general capability for tracking the key finite-rate chemistry effects. Thus whilst successful application has been demonstrated for fire problems that we might expect to begin to challenge the model capabilities (see Hyde & Moss (2003), Welch & Marshall (2003), Paul & Welch (2010)), the assumption is that the method will not prove sufficiently general and will break down for more extreme departures from idealised and well-ventilated fires. Moreover the approach is practically very limited in environments where there are a variety of often complex primary fuel sources, and even less adaptable for cases where there is a significant contribution from decomposing solid-phase materials.

At the other extreme of complexity is the work done with the method of Conditional Moment Closure (CMC) (Clearly & Kent 2005). The CMC approach, independently proposed by Bilger (1993) and Klimenko (1993), offers a solution for the prediction of finite-rate kinetics by using conditionally-averaged quantities to close the chemical production terms. Typically, the species mass fraction is averaged conditionally on fixed values of mixture fraction. By reducing the range of compositions contributing to the mean reaction rate determination, this is effective in reducing the impact of the non-linear variations which result from turbulent fluctuations. The moments of a particular chemical species, conditional on values of mixture fraction, are determined from balance equations which also incorporate the simplifying assumptions of conditioned chemistry. Thus, comparatively complex chemical kinetics can then be included if simple closures are adopted for these source terms, capitalising on the substantially attenuated influence of scalar fluctuations. This approach has been demonstrated to accurately predict the finite-rate kinetics of turbulent hydrogen jet flames (Smith *et al.* 1992) and more recently in simple hood fire problems (Cleary & Kent 2005). However, the improvement comes at a substantial cost, since a further dimension has been added to the problem, thereby requiring solution of sufficient additional transport equations to adequately characterise the conserved scalar space. Thus, whilst very promising, it is likely that computational demands will continue to limit application to simple flame geometries and also to fuels for which reliable reduced kinetic schemes, involving a small number of reactive scalars, are available.

Less computational demanding methods which still decouple the species yields from any assumption of instantaneous chemistry have been proposed by other researchers. One interesting approach is the progress variable method (Pierce & Moin 2004) though this is yet to find application to fire problems. Two other studies seeking to generalise the LES combustion model and RANS flamelet models are described below.

Floyd & McGrattan (2008, 2009) report encouraging progress with use of an extended mixture fraction combustion model with explicit representation of two-step chemistry. This model was introduced in 2007 in version 5 of the Fire Dynamics Simulator (FDS), a code based on Large Eddy Simulation (LES). Here the mixture fraction is decomposed into components representing the three relevant states, i.e. unburnt fuel, partially oxidized fuel (CO) and fully oxidized products (CO_2), thereby allowing a fully consistent approach for the CO chemistry and combustion heat release for very little additional computational expense. The formation step includes an explicit treatment of extinction effects, i.e. CO is only generated in composition space where fuel concentration and temperature exceed a certain threshold, and on the oxidation step a well-ventilated limit value is maintained (i.e. there is no attempt to predict yields under well-ventilated conditions, this is an empirical parameter entered by the user). The predictive capability of the model is first demonstrated for a small-scale slot burner application, using the DNS mode of the model, with predicted species concentrations generally within the 10-20% experimental uncertainty range. For a further case of a reduced-scale enclosure, using the LES model, predictions are within 20-30% of the measurements, with a demonstrable improvement in moving from a one-step chemistry model (Floyd & McGrattan 2009). Results for a wider range of enclosure fires, involving various fuels and fire sizes in the range 15-425kW, showed a greater degree of variability (Floyd & McGrattan 2008) with a tendency towards over-prediction of CO (attributed in part, to the assumed infinitely fast first step for CO formation), and a poorer performance for oxygen containing fuels. Further development is in progress.

Another approach to the problem has been explored by the current authors. We have implemented new models into the SOFIE CFD code (based on the RANS approach), including a “rate flamelet” approach, and a hybrid of this model with a quasi-laminar chemistry model. These approaches are described in more detail in Paul & Welch (2010) but the basic elements are outlined below.

First of all, there is a basic assumption that CO can be treated as a minor species, i.e. its computation is purely post-processed on top of the underlying predictions of an independent combustion model. This approach has the benefit of simplicity, bypassing the complexities of coupled chemistry and heat release, but where CO concentrations become substantial relative to other species additional corrections are required elsewhere, i.e. in heat release and optical properties models for radiation.

CO processes are idealised as a two-step reaction mechanism, i.e. with explicit treatment of formation and consumption, and tracked via a single additional solved variable for CO mass fraction, Y_{CO}. The CO source terms are treated in two rather different ways:

- by neglecting the turbulent fluctuations and adopting appropriate quasi-laminar chemistry, and,
- by constructing flamelets which express the rates of CO formation and oxidation in terms of mixture fraction, i.e. based on the flamelet representation of the underlying combustion process and effecting closure through the 'presumed probability density function (pdf)' transport method, i.e. by integrating over the mixture fraction space.

To facilitate comparisons, and for simplicity, the kinetics adopted for both approaches are taken from the reduced reaction mechanisms for oxidation of hydrocarbon fuels in flames (Westbrook & Dryer 1981), though it would be perfectly possible to use more elaborate schemes in conjunction with a more complex flamelet representation, where available. The rate flamelets are built on top of the existing flamelet models in the SOFIE code, specifically those for methane (Brookes & Moss 1999) and heptane (Welch & Marshall 1999), i.e. the existing state relationships are adopted for all but the CO mass fraction. Thus, for the case of natural gas fuel (assumed to be 100% methane) the source term, $\overline{\rho}\widetilde{S}(Y_{CO})$, is formulated via the two-step semi-global mechanism:

$$CH_4 + \frac{3}{2}O_2 \xrightarrow{R_{CO,form}} CO + 2H_2O$$

$$CO + \frac{1}{2}O_2 \xrightarrow{R_{CO,cons}} CO_2$$

A recommended two-step reaction mechanism for methane (Table IV row 2) describes the instantaneous rates of formation and consumption, respectively, as:

$$R_{CO,form} = 1.5 \times 10^7 \times exp(-30/RT) \times [CH_4]^{-0.3} \times [O_2]^{.3} \text{ mole/(cm}^3\text{ s)}$$

and

$$R_{CO,cons} = 10^{14.6} \times \exp((-40)/RT) \times [CO] \times [H_2O]^{0.5} \times [O_2]^{0.25} \text{ mole/(cm}^3\text{ s)}$$

A reverse reaction is also specified for the oxidation step, with rate:

$$R_{CO,cons} = 5 \times 10^8 \times \exp((-40)/RT) \times [CO_2] \text{ mole/(cm}^3\text{ s)}$$

The latter can be incorporated directly in the formation equation above, since it acts in parallel with the other mechanism.

Other expressions drawn from Westbrook & Dryer (1981) are also investigated (see Paul & Welch (2010) for more details).

Thus the final CO source term for the quasi-laminar model is:

$$\overline{\rho}\widetilde{S}(Y_{CO}) = MW_{CO}\left[\widetilde{R}_{CO,form}(\overline{T},\overline{Y}_i) - \widetilde{R}_{CO,cons}(\overline{T},\overline{Y}_i)\right]$$

where $\overline{Y}_i$ represents the mass fraction of species *i*.

In the rate flamelet model, the Favre-averaged rate, $\widetilde{R}$, is determined from:

$$\widetilde{R}(\widetilde{\xi}) = \int_0^1 R(\xi)\widetilde{P}(\xi,\widetilde{\xi})d\xi$$

where $\tilde{P}(\xi,\tilde{\xi})$ is the β-pdf constructed from the conserved scalar, $\tilde{\xi}$, and variance, $\tilde{\xi}'^2$; $R(\xi)$ is pre-computed from the relevant temperature and species concentrations, all expressed in terms of the mixture fraction, $\tilde{\xi}$, and stored as a flamelet library.

The model is applied to simulation of both the reduced-scale and full-scale enclosure fires referred to earlier. The full-scale enclosure is a standard room with dimensions 2.44 m wide x 2.44 m tall x 3.67 m deep and a 0.76 m wide x 2.03 m tall door centred at the bottom of the front wall (Pitts 1995); the reduced-scale enclosure has overall dimensions scaled to 2/5th size, and the doorway area is scaled according to the $A\sqrt{h}$ enclosure ventilation scaling parameter (Bryner *et al.* 1995). Within the RSE experimental programme over 140 fires were investigated, with heat release rates ranging from 7 to 650 kW, whereas a series of twelve fires ranging from 450 kW to 3.5 MW were completed within the FSE (Pitts 1995). Here we present results only for larger fires, i.e. 500 kW and 3.2 MW, respectively, which are both significantly under-ventilated with global equivalence ratios of approximately 2.52 and 2.58 respectively (Bryner *et al.* 1995).

Results analysis

The results of the new models are compared both with the existing steady laminar flamelet model (SLFM) and against the experimental investigations in reduced- and full-scale enclosures. The predicted temperatures are broadly comparable between the two compartments, and qualitatively similar to the experimental values.

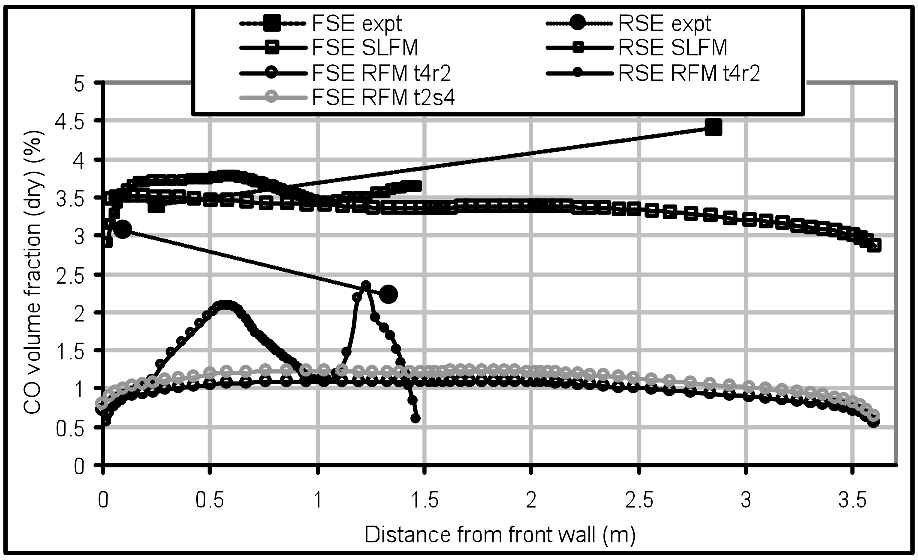

Figure 1. CO yield profiles in the hot layer [Key: experiments (expt), steady laminar flamelet model (SLFM), rate flamelet models (RFM) with kinetic mechanisms from Westbrook & Dryer (1981) Table 4 row 2 (t4r2) and Table 2 set 4 (t2s4)].

Figure 1 shows the comparison of predicted CO yields for the two enclosures with the different flamelet-based models, and including two different mechanisms. The results for the rate flamelet models (RFM) are in both cases lower than the experimental values, whilst the yield flamelets (SLFM) are rather higher and over-predicted for the RSE. The quasi-laminar chemistry predictions (QL) were much higher, quickly approaching the fuel carbon limits which peak at just over 16% towards the centre of the compartment. In the layer, the different rate flamelet kinetics give very similar results. However, the predictions near the layer interface and in the lower layer showed bigger discrepancies for both models, due in part to limitations on the applicability of the mechanisms; the sensitivities to kinetics requires further analysis.

In order to look at the role and impact of choice of chemical mechanisms on the resultant model prediction the influence of a variety of mechanisms for natural gas (proposed by Westbrook & Dryer (1981)) have been further analysed. A summary of kinetic constants is provided in Table 1. The mean cell temperatures and main species concentrations were extracted from the CFD code and used as a basis for examining the sensitivities of the predicted reaction rates. Moreover, artificial variation of the temperature rise has also been explored by means of additional calculations for ±10% cases.

Mechanism	***Label***	***A***	E_a	***a***	***b***
Table IV Row 2	t4r2	1.5×10^{7}	30	-0.3	1.3
Table II Set 2	t2s2	1.3×10^{8}	48.4	-0.3	1.3
Table II Set 3	t2s3	6.7×10^{12}	48.4	0.2	1.3
Table II Set 4	t2s4	1.0×10^{13}	48.4	0.7	0.8
Table II Set 5	t2s5	2.4×10^{16}	48.4	1.0	1.0

Table 1. Reaction rate parameters for methane-air (units cm-sec-mole-kcal-K) Westbrook & Dryer (1981).

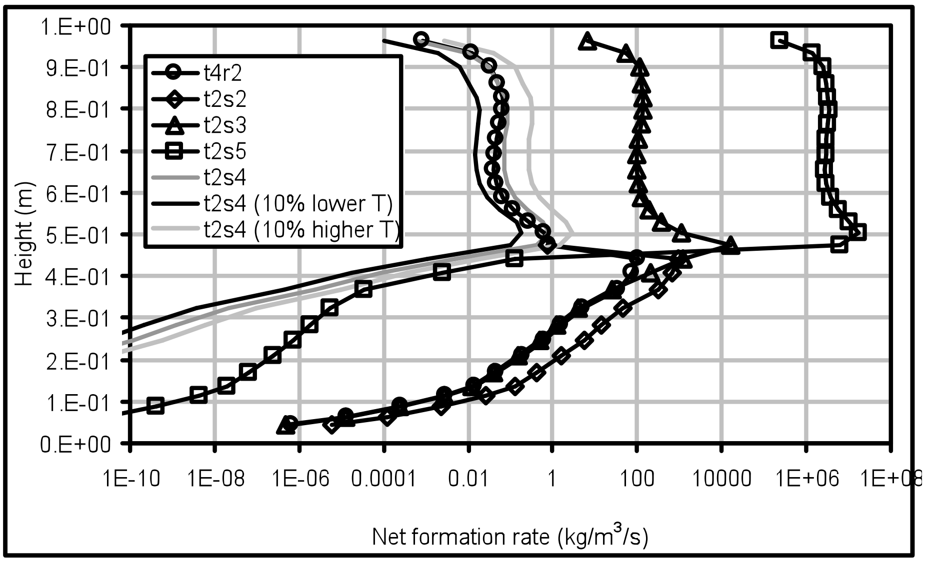

Figure 2. Predicted net CO formation rates against height at the front of the RSE [Key: Westbrook & Dryer (1981) Table 4 row 2 (t4r2) and Table 2 sets 2-5 (t2s2-5)].

From Fig. 2, the two-step mechanism “t2s2”, which when originally derived had given the best agreement with experimental data (fit to flame speeds, Westbrook & Dryer (1981)), is here giving exceptionally high rates in the lower layer, due to the noted negative power in the fuel concentration exponent. Amongst the other options only Set 4 produces reasonable rates for the current application, and it is clear that further investigation of the kinetics used in such models will be required, especially considering this is perhaps one of the simplest of all cases to examine, relating to natural gas.

CONCLUSIONS

The challenge of predicting toxic species concentrations in fire, represented by CO, is presented. Reference is made to the complexities of CO generation, including a variety of phenomena that defy simplistic description by means of correlations, further compounded by the fact that in real fires even the nature of combustibles is often uncertain or poorly characterised experimentally. A range of modelling approaches derived from CFD-based methods are identified, and progress toward the goal of a predictive simulation tool is summarised. It is noted that powerful approaches to accommodating detailed chemistry, such as laminar flamelet models methods, are not well suited to handling the complexity of real fuels, or the finite-rate chemistry which pertains to toxic species production in typical fire environments. On the other hand, more detailed methods which have proliferated in recent years in the wider combustion community, such as CMC, are very computationally demanding and remain primarily in the research domain. Nevertheless, some new treatments based on extended mixture fraction models, or more direct solutions of reduced kinetics in an extension of the flamelet method, do show some promise in providing tractable solutions for fire problems. Much further work on model validation, extending to a greater range of scenarios and fire conditions, is clearly still needed. Moreover, further investigation is required on the reduced chemistry, given the large sensitivities displayed, and this issues also needs to be addressed for more realistic fuels.

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