DEVELOPMENT AND VALIDATION OF A COMPREHENSIVE MODEL FOR FLAME SPREAD AND TOXIC PRODUCTS IN FULL-SCALE SCENARIOS

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INTRODUCTION

Fire hazard calculations require methodologies for prediction of fire growth and flame spread over realistic building materials in full-scale scenarios. If available, a general model capable of estimating the "time-to-flashover" would provide a useful vehicle for evaluation of different methods for reducing the propensity for transition to flashover, thus contributing to development of improved fire safety design. For this purpose, theoretical treatments which are entirely fundamentally-based are precluded due to computational limitations and recourse must be made to some degree of empiricism. Considering the complex range of interrelated phenomena contributing to the overall fire growth and spread, if quantitative accuracy and computational tractability are to be achieved for full-scale applications, care is needed to ensure an appropriate balance between the level of sophistication in the various component sub-models, and between 'empiricism' and 'fundamentals'. This abstract presents an assessment of these issues in the context of a model validation exercise on a series of full-scale tests on real building materials [1].

MODELLING METHODOLOGY

In recent years a variety of flame spread models have been implemented within the framework of an overall approach based on computational fluid dynamics (CFD), e.g. Opstad [2], Yan [3, 4] and Novozhilov [5]. These models are able to capitalize on the detailed information available from the CFD representation of combustion but face similar challenges to any other approach to flame spread prediction in seeking to address the solid-phase pyrolysis. In some cases, the pyrolysis is represented by adopting empirical heat release curves (i.e. cone calorimeter data) whilst others attempt a more fundamentally-based prediction in terms of pyrolysis kinetics. The generality of the former approach can be questioned whilst the applicability of the latter for full-scale scenarios will inevitably be computationally limited.

In addition to the above-mentioned, a range of flame spread models have been implemented in SOFIE, a research CFD code for fire applications, as described in Aksit et al. [6]. The simplest of these models relates time to ignition to an "accumulated net incident flux" parameter which is empirically-derived (see Aksit et al. [7]). This approach can in principle deal with both simple ablating and charring materials and it is relatively undemanding computationally. Despite its empirical nature, the methodology was shown to have interesting potential for representation of fire growth in enclosure fires [7].

In the current study, application of this model has been extended to a variety of realistic end-use scenarios spanning a range of building materials, both cellulosic and plastic-based, with and without flame retardant (FR) [1]. Detailed experimental measurements of flame spread rates, together with overall heat release, temperature, gas species (including carbon monoxide) and smoke were available for model validation. The combustion chemistry and smoke evolution was incorporated in the model by means of a laminar-flamelet approach. Since flame spread rates might be expected to show some sensitivity to the underlying chemistry, and smoke concentrations in particular, availability of such data was invaluable in permitting a detailed assessment of the performance of the fully-coupled model and in identification of the key controlling parameters.

THEORETICAL TREATMENT

Combustion and sooting processes were represented by means of the non-adiabatic laminar flamelet model [8]. For this purpose, flamelets were generated using the CHEMKIN code [9] and the Moss soot model [10] was adopted, together with soot model parameters based on those reported by Moss & Stewart [11].

Flamelets were generated for heptane, a moderately-sooting fuel, using different chemical kinetic mechanisms. The study examined the sensitivity of the flamelet concentrations, and the final model predictions for minor species, to the complexity of the kinetic scheme adopted. It was found that the peak carbon monoxide concentration in the flamelet was about 20% lower using a simple (41 species/274 reactions) reaction mechanism (due to Held et al. [12]) versus a more complex one having 160 species/1540 reactions (due to Seiser et al. [13]). Due to non-linearities, a greater sensitivity was found in overall model predictions for a compartment fire scenario (more than doubled cf. the flamelet difference) so flamelets based on the latter mechanism were adopted for the rest of the study.

For the default heptane-derived flamelet, the value of the soot surface growth constant was calibrated by reference to the measured fuel-dependence of overall soot yields in well-ventilated fires, as reported in the literature [14]. These values were used for all simulations of plastic materials, but it was necessary to multiply the surface growth parameter by an additional scaling factor for the cellulosic materials, which give rise to less soot. The default values were adopted for the other soot model constants [11].

MODEL VALIDATION

Amongst the five different scenarios covered in the test programme [1], the "façade corner-wall" is the simplest in modelling terms, since spread is predominantly concurrent and vertical. This presented the opportunity for calibration of the empirical constants in the flame-spread model for all of the materials. The predictive capability of the model could then be tested in application to the other scenarios. Representative model results are summarised here for two plastic and two cellulosic materials, with one of each being fire-retarded, and for three chosen fire scenarios: the façade corner-wall, the room and the corridor.

Of particular interest is the fact that qualitatively different flame spread behaviours were observed in different tests. In the corridor scenario, the measured horizontal spread along the underside of the ceiling was much more acceleratory than the velocity histories obtained from the other scenarios. It is expected that the comprehensive gas-phase treatment in the CFD code ought to be able to reproduce these different behaviours. Thus, having calibrated some of the more uncertain physical parameters within the scope of the façade corner-wall simulations, the model's predictive capabilities were tested by applying it to the other test cases, *without changing any of the model constants*.

The flame spread parameters used for two plastic materials, a polyisocyanurate foam, coated with Aluminium foil, (PIR) and a fire-retarded extruded polystyrene (EPS), are set out in Table 1. Using about 30000 CFD cells and 2x8 DT rays run times were about 2 hours on a 600MHz workstation.

Fig. 1 shows comparisons between the predicted and experimental measurements of heat release rate, CO concentration and smoke production rates. A reasonable quantitative match has been achieved between prediction and experiment.

The influence of the soot prediction was investigated by running a set of parallel simulations for the PIR case with different values of soot surface growth constant. The results are shown in Fig. 2. It can be seen that the fire growth rate is highly sensitive to the predicted soot concentrations being almost eliminated when soot is omitted from the model. This is expected as the smoke significantly enhances the radiative feedback to the solid surface, which in turn gives rise to greater production of volatiles and higher smoke yields. More detailed study showed that the higher soot concentration did depress temperatures near the fuel surface but that the net effect was an increase in incident flux, giving the enhanced volatilization rates.

The parameters used for two cellulosic materials, a (non-fire-retarded) particle-board and an FR chipboard, are set out in Table 1. In this case, the default heptane soot model required modification, since the volatiles released from cellulosic materials tend to burn much more cleanly than those from purely hydrocarbon-derived products. Thus, the surface growth constant was reduced to 2% of its original value.

Fig. 3 shows comparisons with experiment and agreement is again generally fair. Predicted carbon monoxide concentrations in these cases (not shown) displayed trends similar to those for the plastics though the empirical values were about an order of magnitude lower with the cellulosics. It is thought that the overprediction for this case derives from the heptane chemistry underlying the flamelet combustion model, which is clearly inappropriate for wood volatiles.

Finally, the model was applied "predictively" to the corridor and room scenarios. For the former case, the results agreed very well, qualitatively, with the observed behaviour in the test with prediction of the estimated time to flashover for particle-board linings being only marginally longer (c. 35 seconds) whilst the value for the latter case was only marginally shorter (c. 100 seconds). These simulations confirmed that the model is capable of reproducing the qualitatively different spread behaviour observed in the corridor case very reasonably.

Overall, the model predictions have been shown to be quite acceptable, despite the inherent complexity of the problem. The high sensitivity of the results to the soot concentrations suggests that the predictive capability of the model depends very much on its comprehensive nature. Thus, by implementing a relatively simple flame-spread model, but exploiting the detailed information provided from the full CFD solution, it is found to be possible to obtain realistic predictions of fire growth in representative large-scale scenarios, at relatively low computational cost.

Further work is needed to examine model performance for a wider range of materials and test cases. In addition, the existing flamelet library requires extension, in particular to achieve a better representation of the wood chemistry.

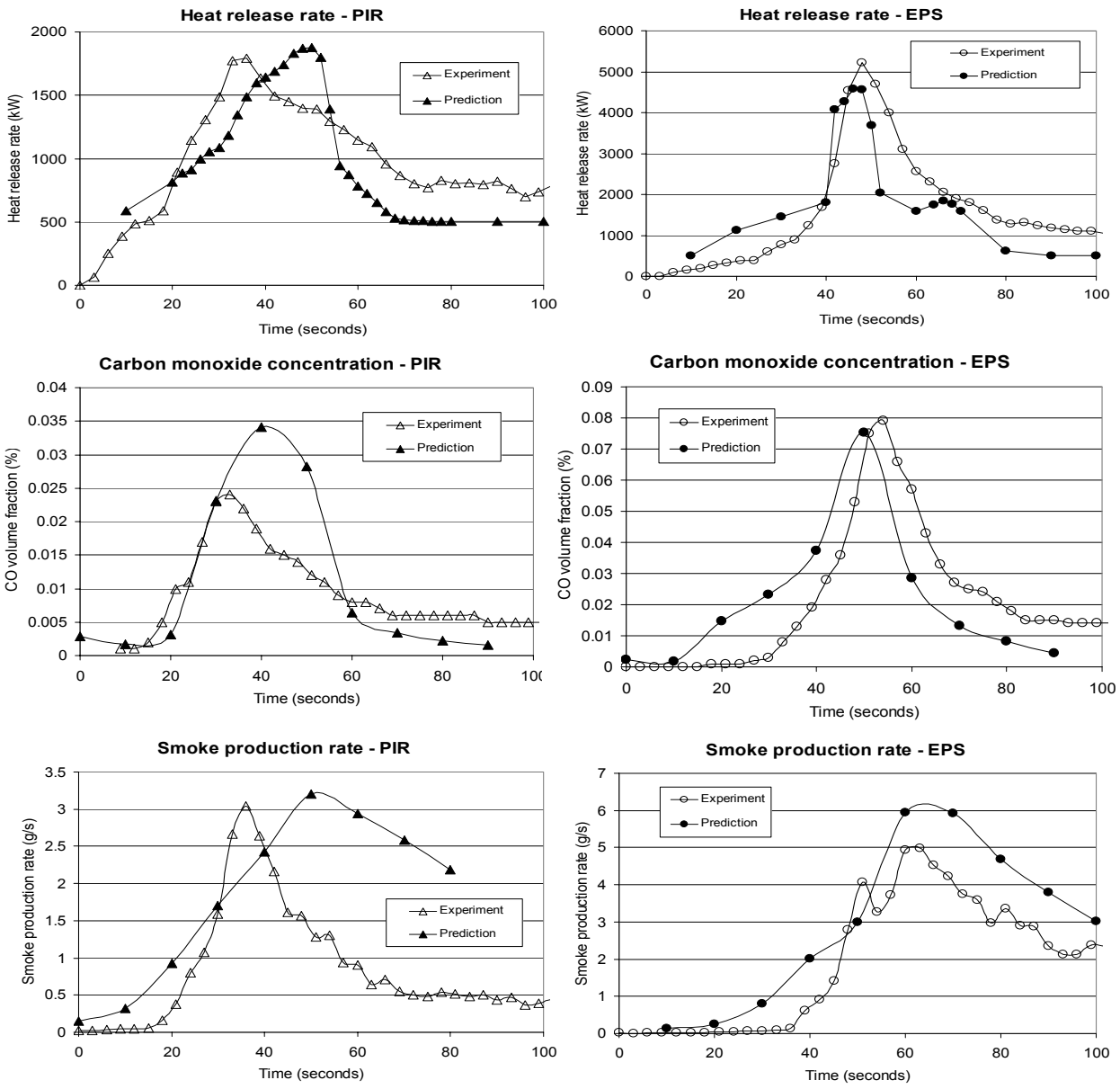

Figure 1 - Comparison of experimental and predicted heat release rates for plastics in corner façade scenario

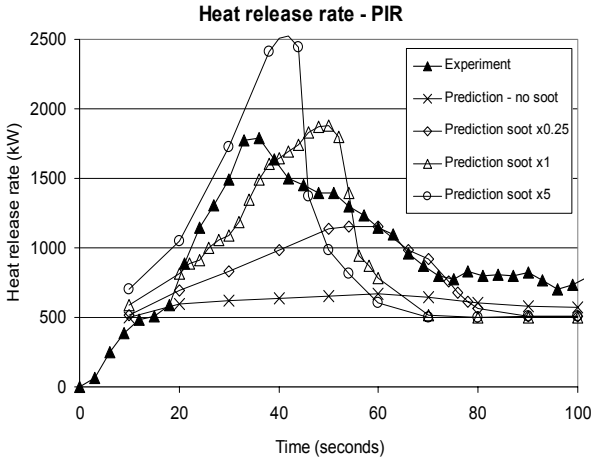

Figure 2 - influence of soot model on predicted spread rate

Parameter	EPS	PIR	Particle-board	FR chip-board
H_{gas} (MJ/kg)	1.3	5.4	1.5	8.0
$q_{acc\ crit}$ (MJ)	0.65	0.45	1.8	1.25
q_{min} (kW/m^3)	5.0	5.0	20	20
hg1	1.0	1.0	1.0	1.0
hg2	0.8	0.8	0.6	1.0
T_{ign} (K)	814	814	685	750
ρ_{vir} (kg/m^3)	37	20	744	780
ρ_{char} (kg/m^3)	20	10	298	165
δ_{char} (mm)	30	25	10	10

Table 1 - flame spread model parameters

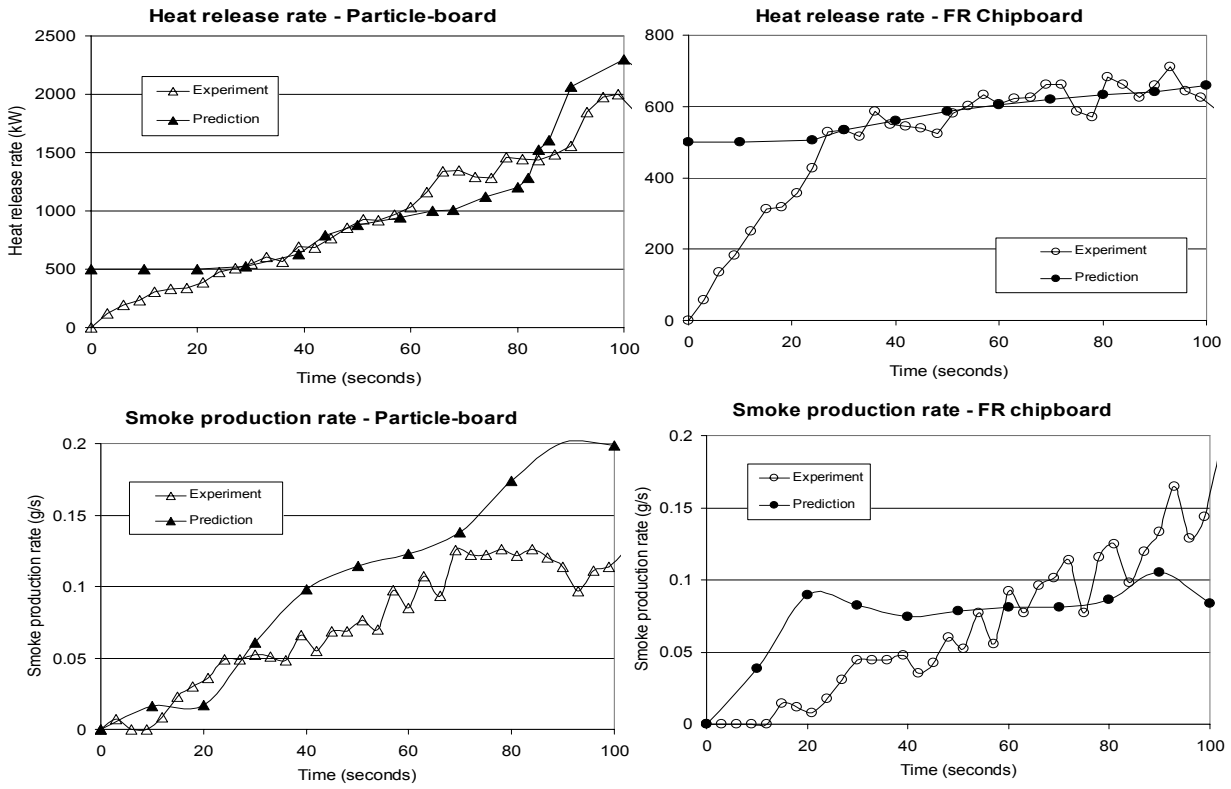

Figure 3 - Comparison of experimental and predicted heat release rates for cellulosics in corner façade scenario

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