# Comparisons of 'Blind Predictions' of a CFD Model with Experimental Data

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## ABSTRACT

This paper presents the first truly 'blind' test of a CFD model used for the prediction of fire conditions in an enclosure. This test formed part of an auditable 'round robin' test of models conducted by CIB W14, sub group 2. The paper demonstrates that CFD models containing the same sub-models as those used in JASMINE are fit for the purpose of predicting gas phase conditions to better than 15% in a flashed over enclosure of the dimensions used here. For accurate prediction of surface heat fluxes in these conditions, however, the quasi-steady one dimensional conduction approximation, satisfactory for smoke movement problems, is not adequate.

**KEYWORDS:** CFD, field model, JASMINE, validation, verification, blind prediction, CIB

## INTRODUCTION

Modern computational fire models have been under development for at least two decades. Over that period they have graduated from being research test vehicles and prototypes to now enjoying increasing utility as essential tools for the practising engineer. This development has been encouraged largely by the trend towards performance-based regulation and its reliance on engineered approaches to achieving fire safety.

Furthermore, there has been a growing confidence in the ability of modelling. However, although most current models have been developed by continuous comparison with experimental data there has, until only very recently, been no auditable check of the ability of models to predict conditions in experiments for which the data are not known. Although there have been several modelling 'challenges' undertaken by the fire community [e.g. 1,2], none has, as far as the authors are aware, been truly 'blind'. Thus the criticism can be made, sometimes with justification, that models have been 'tuned' to obtain agreement with data.

In order to obtain an objective assessment of the capability of current models, the Fire Commission of the International Council for Research and Innovation in Building and

Construction (CIB W14) has been co-ordinating a 'round robin' programme of comparisons of model predictions against experimental data [3]. These data were not made available to those involved in modelling the experiments until after submission of their predictions.

Only the geometry, boundary conditions and fire source information were supplied initially. After submitting their predictions to the CIB co-ordinator, the experimental measurements were then released to the 'round robin' participant. The predictions were then compared against the measurements and comments provided. The participant was at this stage free to perform further simulations, but now with knowledge of the data.

The 'blind testing' of one particular model as part of this 'round robin' exercise is the subject of this paper. The model is JASMINE, a 'field' model which has enjoyed a long pedigree of comparison with data, reported for example in earlier of these conferences [4-7] and elsewhere, but none of it 'blind' and audited in the sense of this work. Furthermore, most of that work concentrated on well-ventilated smoke movement problems. The test case described here reaches ventilation-controlled conditions.

## CFD MODELLING

Fire models based on computational fluid dynamics (CFD) have been described in detail elsewhere [e.g. 8]. Based on first principles, they solve the fundamental transport equations for mass, momentum, enthalpy and species concentrations. This ensures that all the important physical and chemical processes and their interactions, describing the production and movement of smoke, are simulated implicitly.

These rigorous transport equations call upon sub-models to describe the complex processes of turbulence, combustion and thermal radiation. Furthermore, approximations are generally employed for the treatment of heat and momentum transfer to the enclosure boundaries and in the numerical discretisation of the continuous partial differential equations. It is these approximations and sub-models that are the primary subject of any validation and verification exercise.

Issues of validation and verification have become increasingly important for the wider CFD community, which is concentrating primarily on solutions of the isothermal Navier Stokes equations [e.g. 9]. When applied to fire problems additional questions associated with those sub-models unique to fire need to be considered. These more philosophical issues will not be discussed here but will need to form the basis of 'best practice' guidance that should result from the 'round robin' exercise.

## EXPERIMENT DETAILS

The experiment for the model evaluation reported here was one of a series performed in the 1980s in the VTT testing hall in Finland, the results from which were not published. Two wood cribs were located inside an enclosure containing a single high level slot opening. One of these cribs was ignited and fire was allowed to spread from the first to the second crib.

Figure 1 shows the geometry of the enclosure and the location of the cribs. The location of ignition of the corner crib is indicated. This was the only ignition point. Fire spread naturally to the second crib as a result of the developing conditions inside the enclosure. Each crib was constructed from 0.04 m x 0.04 m softwood battens, with a volume ratio of one part wood to one part air. The enclosure walls and ceiling were constructed from low-density concrete block. The specific heat, thermal conductivity and density of this aerated concrete block were 1050 J $kg^{-1}°C^{-1}$, 0.12 W $m^{-1}°C^{-1}$ and 500 kg $m^{-3}$ respectively.

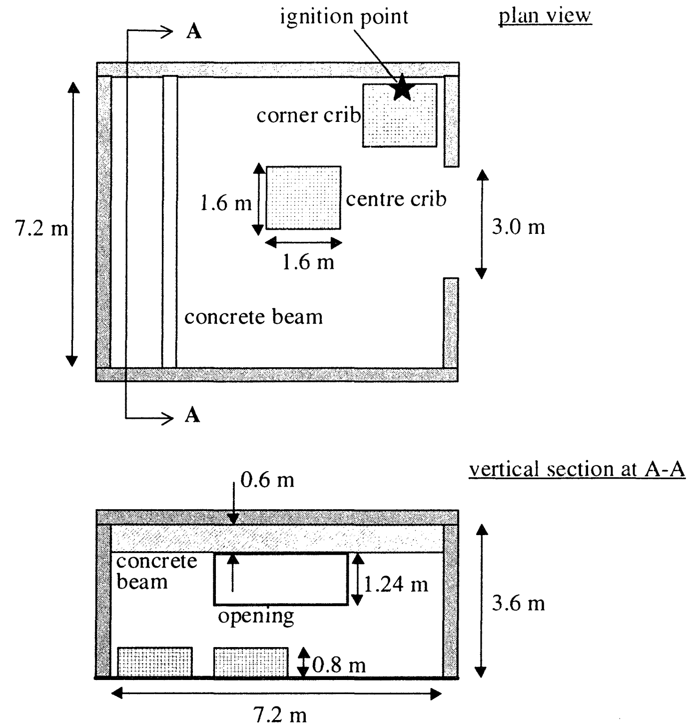


FIGURE 1 Geometry of the experiment

A concrete beam, 0.6m deep, was included under the ceiling as shown in Figure 1. The walls and ceiling were 0.3 m thick.

Other than the geometry and wall materials, the only information supplied for the blind simulations was the measured individual mass loss rate for each crib together with an effective heat of combustion. Mass loss rates were determined from the raw weight loss data through which a smooth curve had been fitted and time derivatives determined. Figure 2 shows the resultant mass loss rates for the two cribs.

The two-hour duration of the experiment made the computational load for CFD models particularly great. However, this did provide a good test of numerical stability.

Prior to the blind simulation, a suggested effective heat of combustion was provided. This was a product of a 'burning efficiency' factor $\chi$ and a constant heat of combustion $\Delta H_c$, assuming the values 0.7 and 1.78 x $10^7$ J $kg^{-1}$ respectively. This approach was without doubt an over-simplification, and the consequences of this are discussed later.

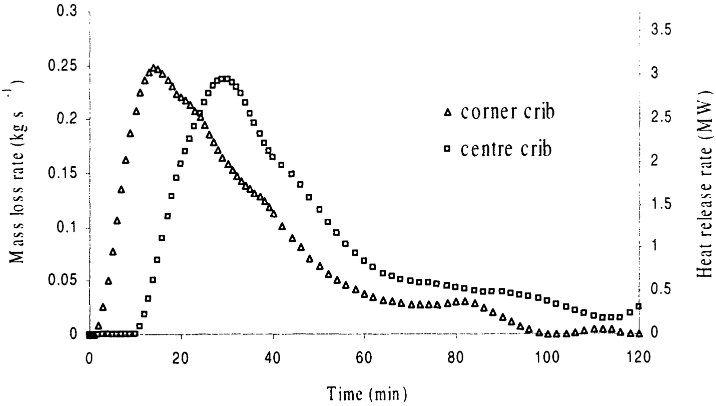


FIGURE 2 Mass loss and heat release rates of the two wooden cribs

The heat release rates obtained by multiplying the mass loss rates by $\chi \Delta H_c$ are shown on the right hand scale of Figure 2.

## MODEL DETAILS

JASMINE is a three-dimensional finite-volume code using a single-block Cartesian mesh and a variant of the SIMPLE pressure-correction algorithm. Convection terms are discretised with the first-order 'upwind' scheme and time advancement is by the first-order, fully implicit, backward Euler scheme. Turbulent closure is by a $k$-$\varepsilon$ model using the standard constants and additional buoyancy source terms. Standard wall functions for enthalpy and momentum are used to describe the turbulent boundary layer adjacent to solid objects. More detail has been given in references 4-8.

The crib combustion process was modelled in this study using a simplified one-step chemical reaction for cellulose.

$$CH_2O + O_2 \rightarrow CO_2 + H_2O \qquad (1)$$

The heat of combustion ($\Delta H_c$) was set to the suggested value of 1.78 x $10^7$ J $kg^{-1}$, and the 'efficiency' factor (0.7) was incorporated instead into the definition of the effective mass burning rate $\dot{m}$.

$$\dot{m} = \chi \dot{M} \qquad (2)$$

Here $\dot{M}$ is the mass burning rate estimated from the experiment data (Fig 2).

The local gas phase reaction rate was calculated from the modified version of the eddy break-up mixing model as summarised for example by Cox [8]. Complete oxidation of the fuel was assumed when sufficient oxygen was available, and therefore predictions of carbon monoxide were not provided. However, given the conditions inside the enclosure, a significant production of $CO$ may be expected. The predicted $CO_2$ concentrations can be taken to provide an approximate measure of the combined $CO_2$ and $CO$ concentrations.

It would be very demanding of any model to simulate the burning cribs in detail, especially if the surrounding enclosure is to be modelled too. To simplify matters in the simulations, the wood cribs were included as solid blockages with the same horizontal cross-sectional area as in the experiment, but only half the height. The fuel was then 'released' uniformly from the top surface of each blockage.

Radiant heat transfer was modelled with a six-flux model, which assumes that radiant transfer is normal to the co-ordinate directions, ignoring the angular dependence of radiant intensity. Local absorption-emission characteristics of the combustion products were computed by using Truelove's mixed grey-gas model [see, for example, 8].

JASMINE calculates the heat fluxes at the solid surfaces. Whereas the convected and radiated fluxes are generated by the CFD and radiation models, the conducted flux into the solid is calculated using a quasi-steady one-dimensional approximation. A steady state condition is imposed on the conducted flux $\dot{q}''_{con}$ so that

$$\dot{q}''_{con} = -k_w \frac{\Delta T}{\Delta x} \tag{3}$$

Here $k_w$ is the thermal conductivity of the solid material and the temperature gradient $\Delta T/\Delta x$ takes a constant value between the surface and a distance $\delta$ below the surface, referred to as the thermal penetration depth. $\Delta T$ then takes the value $T_s$-$T_o$ where $T_s$ and $T_o$ are the surface temperature and the initial solid temperature (ambient in this case) respectively.

The thermal penetration depth is given approximately by the expression

$$\delta = 2\left(\frac{k_w t}{\rho_w c_w}\right)^{1/2} \tag{4}$$

Here $\rho_w$ and $c_w$ are the density and specific heat of the solid respectively and $t$ is the time from ignition.

Surface temperatures are calculated by balancing the convected and radiated fluxes with the conducted flux into the solid, yielding a non-linear equation for surface temperature. This is solved iteratively.

Unfortunately, the corner crib had been incorrectly located in the problem specification for the 'blind' simulation. In the experiment, the crib had been located diagonally opposite the corner actually specified - see Figure 3. The full transient results presented here are for this incorrect specification.

Some steady state simulations were therefore performed later to examine the consequence of using this incorrect location for the corner crib. For these simulations, a time from ignition of 30 minutes was assumed with the heat release rates of the two cribs fixed at their corresponding values at that time, so that the total heat release rate of 4.9 MW was close to its peak value. These simulations indicated that the gross features of the solution were not affected unduly by the incorrect specification of the corner crib location. In particular, the species concentrations near the centre of the ceiling remained almost unchanged, although the temperature predictions were typically 50-100 °C lower with the crib in the correct location. This has some implications when comparing prediction against measurement, and this is discussed later.

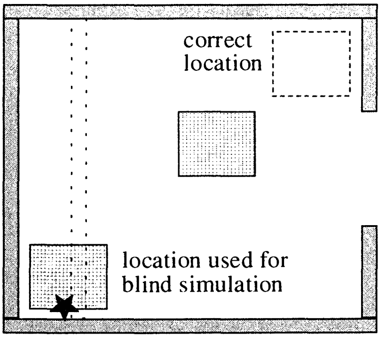


FIGURE 3 Location of corner crib in the blind simulation

The experiment was modelled using a mesh of 46,080 cells. This represented a balance between the need for fine resolution to capture correctly the entrainment and heat transfer processes and the demands of simulating the two-hour duration of the experiment. On an Alphastation 500 (333 MHz processor) with 256 Mbytes RAM, the two-hour experiment took just under three weeks to simulate. The minimum cell dimension of 0.075 m was used for the cells next to solid boundaries, while the maximum cell dimension inside the enclosure was 0.55 m. This mesh is referred to as the 'standard' one in the mesh refinement discussion below.

A mesh sensitivity analysis was performed with steady state simulations using the original mesh and a double resolution mesh, i.e. a total of 368,640 cells (eight times the number of cells in the original mesh). As for the steady simulation above, an elapsed time of 30 minutes was assumed for these comparisons, with the heat release rates of the two cribs fixed at their corresponding values at 30 minutes, i.e. 2.9 MW and 2.0 MW for the centre and corner cribs respectively. The solutions achieved with the two meshes were very similar, indicating that the standard mesh was acceptable for the full transient simulation. Table 1 illustrates the similarity between the two solutions for a selection of criteria.

The free (ambient pressure) boundaries were placed well away from the vent opening. They were located 9m above the compartment ceiling in the vertical direction and 7.4m from the compartment wall containing the vent.

All experimental measurements specified in the blind-simulation design report [3] were predicted with the exception of $CO$ concentration. The predicted values were recorded at one-minute intervals although the numerical time-step used was two seconds throughout the simulation.

TABLE 1. Comparison of standard and fine mesh solutions

| **mesh** | **$T_{b1}$ temperature** (°C) | **maximum** $m_{pr}$ | **maximum surface radiation flux (kW $m^{-2}$)** | **mass flow into opening (kg $s^{-1}$)** | **convected heat out of opening (MW)** |
|---|---|---|---|---|---|
| 'standard' | 1141 | 0.368 | 22.6 | 1.87 | 2.61 |
| 'fine' | 1157 | 0.368 | 23.2 | 1.97 | 2.52 |

(Here $m_{pr}$ is the combustion product ($CO_2 + H_2O$) mass fraction)

## COMPARISON OF MEASUREMENTS AND PREDICTIONS

The experiment measurements were:

i) Temperatures from three thermocouple columns, at locations $T_a$, $T_b$ and $T_c$ in Figure 4. Each column contained 11 evenly distributed thermocouples.

ii) Species concentrations ($O_2$, $CO_2$ and $CO$) at a location 0.3 m below the centre of the ceiling. The gas was 'dried' prior to measuring the species volume fraction.

iii) Conducted fluxes into the solid at the wall and ceiling surfaces at the four locations $F_1$, $F_2$, $F_3$ and $F_4$ shown in Figure 4. These fluxes were estimated from temperature readings from thermocouples embedded at various depths in normal density concrete castes that were bored into the aerated block. The ratio $(k\rho c)^{0.5}_{normal}:(k\rho c)^{0.5}_{aerated}$ was approximately 5:1.

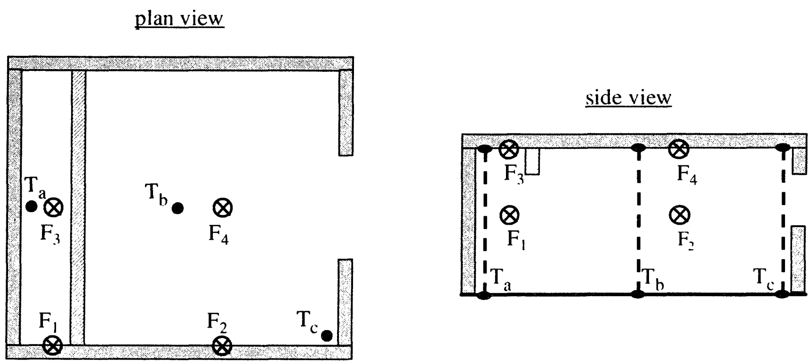


FIGURE 4 Location of thermocouple columns and surface flux measurements

Figures 5 to 10 show comparison plots for the following selection of these measurements:

i. Species ($CO_2$ and $O_2$) volume fractions 0.3 m below the centre of the ceiling.
ii. Gas temperature 0.3 m below the ceiling at the $T_a$, $T_b$ and $T_c$ thermocouple columns ($T_{a1}$, $T_{b1}$ and $T_{c1}$).
iii. Gas temperature 1.8 m above floor level at the $T_b$ thermocouple column ($T_{b6}$).
iv. Gas temperature 0.9 m above floor level at the $T_a$ and $T_c$ thermocouple columns ($T_{a9}$ and $T_{c9}$).
v. Surface fluxes at the $F_1$ and $F_2$ locations.

Both measurement and prediction show that flashover conditions develop during the first ten minutes or so. The gas temperature measurements reveal, see Figures 7-9, that the hot gas layer was 'well mixed' and extended down to floor level throughout the enclosure around 20 minutes from ignition. This 'single zone' characteristic of the experiment appears to be the main reason that the error in the location of the corner crib had only a second order effect on the results.

With the exception of a temporal shift, seen in Figures 5-10, the predictions are in reasonably good agreement with the measurements. The overall qualitative behaviour of the experiment is captured, with the development of flashover conditions predicted correctly. The main discrepancies are in the peak gas temperatures and peak boundary heat fluxes.

The predicted and measured values for $CO_2$ and $O_2$ volume fractions are in good agreement, indicating that the combustion model has coped successfully with the oxygen reduced flashover conditions. There is a noticeable discrepancy in $CO_2$ concentration during the decay phase of the experiment. However, the experimental value of 5% seems high, particularly since the $O_2$ concentration has returned to its ambient condition. One must question the measurement here and also the apparent $O_2$ saturation at 5%, during the period of peak heat release, whilst the $CO_2$ concentration continued to rise. These observations highlight the need to examine the accuracy of the experimental measurements as well as the predictions when making comparisons of this kind.

Gas temperatures, however, have been over-predicted during the intense flashover stage of the experiment by between 100 °C and 200 °C (about 15%) depending on thermocouple location. The biggest discrepancy between prediction and the measurement, however, is in the heat fluxes into the solid structure, with the predicted peak fluxes being only approximately half the measured values. This in turn provides one explanation for the predicted peak temperatures being greater than the measured values, the reasoning being that if more heat were lost to the solid structure then the gas temperatures would be reduced. Again, further analysis of the flux differences, and the implications of employing a fixed combustion efficiency on gas temperature, are provided later.

The temporal shift we speculate to be closely related to the absence in JASMINE of a moisture release model for wood.

## DISCUSSION

The overall agreement between prediction and measurement is good. There is, however, one serious discrepancy concerning the treatment of boundary heat fluxes.

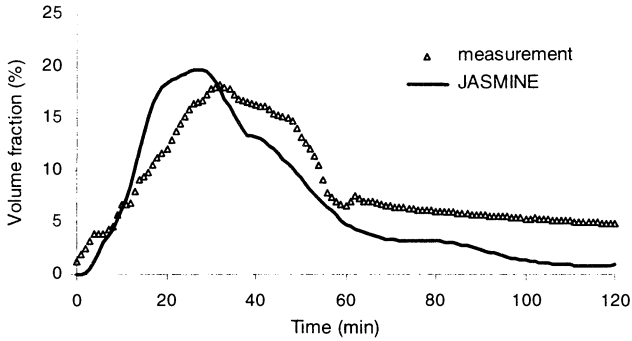


FIGURE 5 $CO_2$ volume fraction

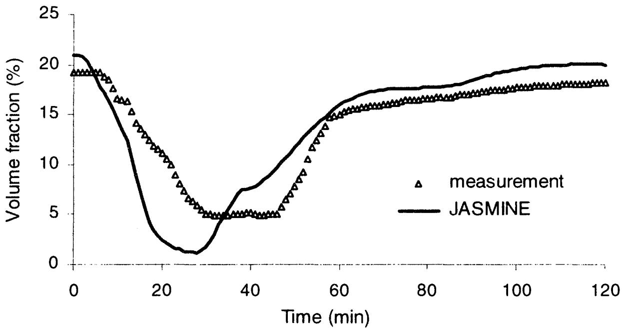


FIGURE 6 $O_2$ volume fraction

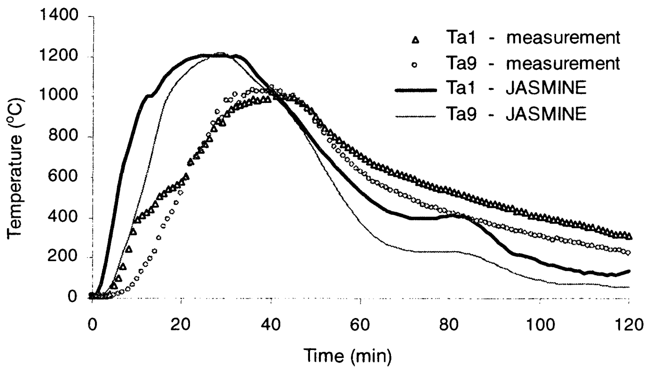


FIGURE 7 $T_a$ temperatures

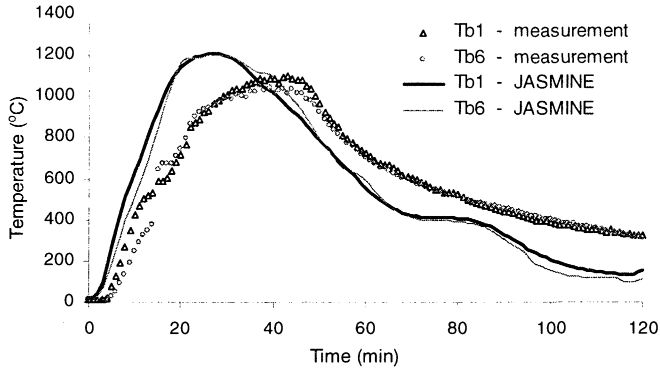


FIGURE 8 $T_b$ temperatures

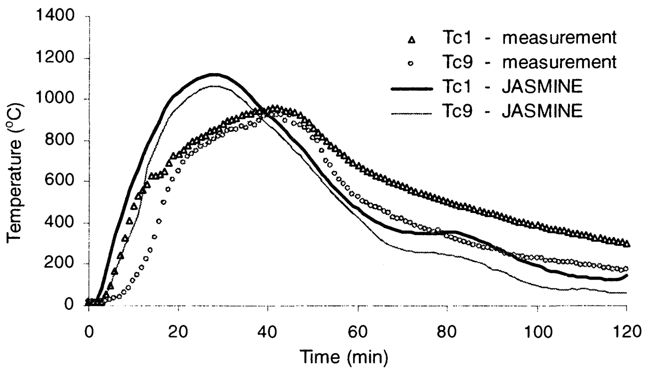


FIGURE 9 $T_c$ temperatures

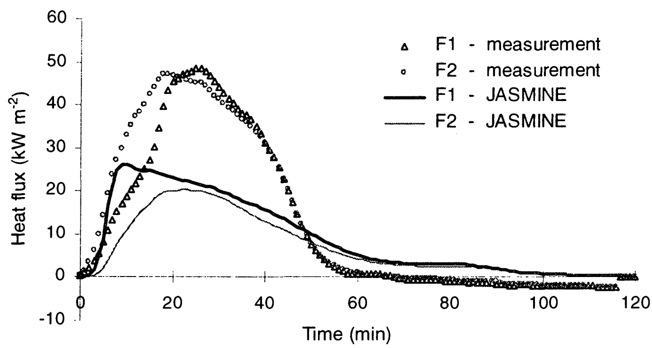


FIGURE 10 Surface fluxes from gas to 'normal' density concrete bores

The 15% over-prediction of peak gas temperatures can be attributed to the predicted boundary fluxes being too low. This was confirmed in some additional steady state simulations with the crib heat release rates fixed at their values after an elapsed time of 30 minutes. By applying fixed-flux thermal boundary conditions at the walls and ceilings at double that determined by the one dimensional conduction approximation, as suggested by Figure 10, the gas temperatures inside the enclosure were reduced by between 100 °C and 150 °C.

As noted earlier, even for transient simulations, JASMINE uses a quasi-steady assumption for the conduction losses. Even if the thermal penetration depth is calculated correctly, the linear temperature gradient imposed by the quasi-steady assumption will yield a surface flux that is too low. The temperature gradient below the surface will in reality be steeper, yielding a greater conduction loss. The importance of this approximation had not been apparent in our earlier studies of the pre-flashover phase of fire growth.

Another serious influence on the predictions was the proposed constant effective heat of combustion ( $\dot{Q}_{eff} = \chi \Delta H_c \dot{M}$ ) in the original specification. A measurement of this property, using oxygen depletion calorimetry, was later made available, and is shown in Figure 11. This shows clearly that the constant assumption incorrectly allows too much heat to be released during the earlier stages of the fire (up to around 35 minutes) but too little during the decaying phase (after 80 minutes).

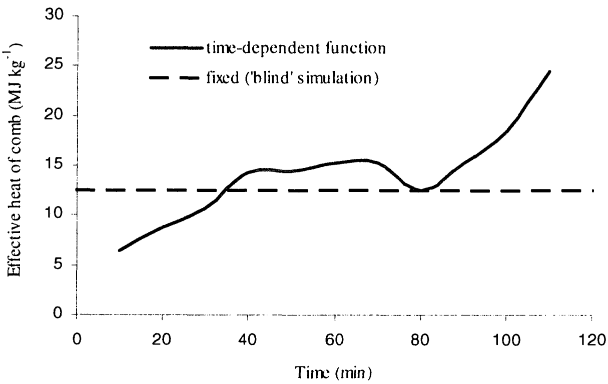


FIGURE 11 Measured heat of combustion as a function of time

## CONCLUSIONS

What has been reported is, we believe, the first truly 'blind' test of a CFD model used for the prediction of fire conditions in an enclosure, as recommended at a CIB fire modelling workshop in 1987 [10]. The scenario chosen has been particularly challenging because it includes two separate fire sources and flashover conditions prevail for a period of about 20 minutes.

Although the results from only one CFD model are reported here there is the clear conclusion that is likely to be valid for all models, both CFD and zone, that the quasi-steady one dimensional conduction approximation is not appropriate for the severe conditions of this fire.

It would appear that this CFD model and others that adopt similar sub-models are fit for the purpose of predicting gas conditions within compartments of this size to within at least 15%. What they are not fit for, with the conduction approximation employed here, is accurate prediction of surface heat flux in post-flashover fire conditions. This short-coming, not apparent in smoke movement studies involving lower temperatures, should be straightforward to rectify and indeed some CFD models, e.g. SOFIE [11], already calculate conjugate heat transfer through the gas-solid phase interface without using the approximation.


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