The Effect of Model Parameters on the Simulation of Fire Dynamics

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Abstract

The sensitivity of computer fire modelling using results from NIST’s Fire Dynamics Simulator (FDS) to a set of input parameters related to fire growth has been analyzed. The scenario simulated is the real-scale Dalmarnock Fire Test One and the modelling results are compared to the measurements. Fire size and location, convection, radiation and combustion parameters were varied in order to determine the associated degree of sensitivity. Emphasis is put in the prediction of secondary ignition and time to flashover. In this context and while keeping the HRR constant, simulations of fire growth are significantly sensitive to location of the heat release rate (HRR), fire area, flame radiative fraction, and material thermal and ignition properties. The simulations are relatively insensitive to the heat of combustion (while keeping the HRR constant), the soot yield and the heating from the smoke layer. The results indicate that the future development of successful fire forecast methodologies of fire growth using CFD must focus on the global HRR as well as the important parameters identified here.

Key words:
FDS, prediction, Dalmarnock, modelling, forecast

Nomenclature

<table>
<thead>
<tr>
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<th>Description</th>
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</thead>
<tbody>
<tr>
<td>α</td>
<td>Absorptivity</td>
</tr>
<tr>
<td>δ</td>
<td>Thickness m</td>
</tr>
<tr>
<td>ε</td>
<td>Emissivity</td>
</tr>
<tr>
<td>ρ</td>
<td>density [kg/m^3]</td>
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<tr>
<td>σ</td>
<td>Stefan-Boltzmann constant [kW/m^2·K^4]</td>
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<table>
<thead>
<tr>
<th>Superscripts</th>
<th>Description</th>
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<tr>
<td>′′</td>
<td>Per area [1/m^2]</td>
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1. Introduction

The central aspect of fire protection engineering is to understand the dynamics of compartment fires in order to design built environments where the likelihood of a fire event is minimized and the protection of its people, content and structure from fire damage is maximized. Fire safety aims at constantly improving and developing new response systems for these emergencies. A possibility currently being explored in new emergency response systems is to combine live sensor monitoring and forecast of fire development [1]. It is envisioned that the forecasting of fire dynamics in enclosures will imply a paradigm shift in the response to emergencies, providing the fire service with essential information about the fire ahead of time [1, 2].

There is an inherent difficulty in predicting fire behaviour since it involves complex dynamics driven by critical events, such as the ignition of secondary items, flashover, window breakage, sprinkler activation, etc. Moreover, fires involve mechanisms that develop in length scales ranging from millimeters to meters, and time scales from milliseconds to minutes. Coupled computational simulations of these phenomena (i.e. CFD) demand extensive computational times that are far greater than the time associated with the phenomena themselves. Thus, a forecasting emergency response technology is currently non-existent because, putting aside the level of accuracy attained, the best available fire simulations predict with a negative lead time, i.e. the fire evolves at a much faster rate than forecasts can be produced. If comprehensive computational models are to be used to estimate, forecast and understand fire growth in support of emergency response, a simple, robust and effective approach is required.

The most promising technology for fire forecasts involves the constant update from live-recorded data to assist the simulations. If available in real time, sensor data could be used to train and correct the simulation output. One of the current main
limitations for this technology is in the large number of parameters that are required in fire models. Many of these parameters are scenario dependant, poorly defined or unphysical and the majority is associated to large uncertainties. Thus, for the concept of fire forecast to work and in order to be able to actually predict fire dynamics ahead of time, it is essential to identify the parameters to which fire modelling is most sensitive, so that these become the centre of attention of the forecast process.

2. Large-Scale Tests and Simulations

Only a few real-scale fire tests in enclosures have been conducted and very few of them had the required level of instrumentation for field model comparison; the BRE large compartment test series [3], NIST’s experiments for the World Trade Center (WTC) [4] and The Dalmarnock Fire Tests [5] to name the most important. All these have been the objective of fire modelling. The BRE test series were modelled by Pope et al. [6] with FDS and a reasonable agreement was reached within the context of structural fire safety, although their post-flashover simulations underpredicted the measured temperatures. The NIST experiments of fire growth were primarily conducted to validate their WTC simulations with FDS [7]. The Dalmarnock Tests, the most recent, have been modelled a priori [8] and a posteriori [9] and are the focus of the simulations in this paper.

The Dalmarnock Fire Tests involved two flats in a 23-storey reinforced concrete tower in Glasgow (UK) and were conducted in July 2006. Test One was held in a two-bedroom single family flat, with the living room set up as the main experimental compartment as shown in Fig. 1. Extensive information on the layout, experimental setup and outcome of the Dalmarnock fire tests can be found elsewhere [5, 10], but an overview is included here for quick reference.

A large number of sensors were installed throughout the flat in order to monitor in detail the fire development [5, 10]. Dalmarnock is the only fire test to date with an instrumentation density high enough to provide measurements with spatial resolution suitable for comparison with field models. More than 270 thermocouples were distributed in the main compartment to measure gas temperatures. 20 video cameras produced visual recordings which allowed monitoring of the fire development. Other measurements include light extinction, gas velocities at the opening, smoke detectors, temperature and heat fluxes on the walls and monitoring of the structural response of the building.

The fire in the Dalmarnock Test One was initiated at the sofa near the corner away from the window of the fire compartment (see Fig. 1). The sofa fire grew and after 275 s ignited the plastic boxes on a bookshelf standing about 1 m away. Once the bookshelf caught fire and flames spread vertically, the smoke layer descended rapidly to the ground and flashover took place at 300 s. At 800 s the compartment window was purposely broken from outside and led to a change in the ventilation conditions. Finally, 1140 s into the fire, the fire brigade intervened and extinguished it.

Two sets of CFD simulations have been carried out regarding the Dalmarnock Fire Tests. Before the tests actually took place, a round robin study was conducted with the objective of assessing the capability of blind predictions of real fire scenarios [8]. The output from the simulations of the participating teams scattered over a wide range of values and no consistency between simulations and the measurements was established beyond mere qualitative trends. The results showed that blind a priori simulations of complex scenarios are not accurate and thus that fire forecasts using these tools alone are not reliable. A posteriori simulations using FDS version 4 aided by the experimental measurements were carried out after the tests [9]. These show that even when full access to measurements is given, it is remarkably difficult to reproduce the spatial patterns and the different stages of fire development to a satisfactory level of accuracy.

In this work, further a posteriori simulations using FDS version 4 have been carried out using the experimental measurements. The objective is to find a set of model parameters that allow reproducing well the pre-flashover fire. In the process of attaining accurate results, it is possible to identify the variables to which the output is sensitive and those parameters that have a minor effect in the result. This sets a framework for the development of simpler models that could potentially achieve positive lead times within the required levels of precision.

3. Fire Dynamics Forecast and Model Parameters

Fire dynamics are fundamentally different during the pre- and post-flashover phases of a fire. The dynamics of each phase is thus associated to different modelling parameters. This difference suggests splitting the problem in two parts.
3.1. Pre-flashover Fire

During the pre-flashover period the fire is growing and localized, i.e. only a few items within the compartment are burning and the production of pyrolyzates is the limiting step [11]. Fire growth is generally driven by flame spread over the initially burning item or secondary ignitions of surrounding objects. Eventually, if sufficient objects are burning, flashover could take place. From the point of view of fire forecast, knowing the flame spread and which of the items in the room will ignite next, and the time of this ignition allows predicting the time to flashover. Secondary ignition is controlled by the heating of material surfaces by the flame and the hot layer. Thus, if the location of the fire and the rate of heat release could be estimated based on sensor data (e.g. from thermocouples and heat flux gauges on the walls and ceiling of the compartment) then once the flame location and height is known, the heat fluxes to surrounding surfaces and their temperature evolution could be calculated. This would allow prediction of the time to ignition of different items. This work studies the sensitivity of simulated surface temperatures and incident heat fluxes during the growing fire phase to different parameters.

3.2. Post-flashover Fire

Once flashover has occurred the fire is no longer localized, and combustible gases fill the entire compartment. They will burn when they find the right conditions of oxygen concentration and temperature. Post-flashover fires are ventilation controlled, and thus from the point of view of fire forecast, knowing the ventilation conditions is essential for accurate predictions. One of the most challenging parts is that the fire could lead to window breakage that could modify substantially the fire behavior but are difficult to predict with current tools. The effect of fire parameters during post-flashover stage are beyond the scope of this work and will be subject of future studies.

3.3. Model Parameter

The most important input variable to fire simulations is the evolution of heat release rate (HRR) with time [12, 13]. However, in real fires the HRR is seldom available and can only be estimated at best. Only experiments conducted under controlled laboratory conditions provide measurements of HRR evolution. Current fire modelling tools provide good predictions of the thermal effects of a fire (e.g. the resulting thermal environment) but the predictions of the fire development are poor (e.g. flame spread and fire growth). The proper prediction of the HRR evolution is therefore among the first priorities of a fire modeller studying real fire development. The effect of the modelling parameters to predict the HRR evolution is studied here.

In general terms, there are three different types of parameters that can be varied in a CFD simulation. The first type consists of parameters related to the boundary conditions, such as geometry, openings and the location of solid items. These parameters are the basis of any simulation and in principle are determined by the fire scenario that is to be modelled. Thus their uncertainty is related directly to the confidence in the known details from the scenario geometry. The second type consists of the parameters related to physical properties of the fuel packages and other solid surfaces such as thermal inertia, ignition temperature, heat of combustion, surface emissivity, etc. In theory, these parameters can be experimentally measured or determined via empirical correlations, but in practical terms the associated uncertainty can be very large creating a wide range of possible values. Mathematical and computational parameters comprise the third type of parameters and generally depend on the model being used. In the case of LES, the grid size, the Smagorinsky constant and others belong to this group of parameters [14]. These parameters do not have any physical meaning and are related to mathematical approximations and the solution method of the particular model. Nevertheless, variation of those parameters affects the outcome of the computations. In principle, their values should be determined based on computational and mathematical criteria alone and calibration. These parameters have been the focus of many studies, e.g. Wen [15].

This paper focuses mainly on the effect of the second type of modelling parameters, the material properties, but the other types are also investigated.

4. Results of Sensitivity to Model Parameters

The results of simulating the Dalmarnock Fire Test One are presented in this section. Simulated gas phase temperatures are compared to the measurements from ignition to 250 s (before flashover), and surface temperatures on the bookshelf next to the sofa obtained from simulations for different parameter values are presented.

4.1. Ignition Source

A typical love-seat sofa acted as an ignition source for the Dalmarnock Fire Test. It was ignited using a waste paper basket standing adjacent to it. A cotton blanket was placed over the armrest of the sofa with one part hanging inside the basket. Over both the basket and blanket, 300 ml of heptane were poured to ensure ignition.

Prior to the large-scale test, a sofa replica was burned under laboratory conditions in a furniture calorimeter [16]. Figure 2a shows the HRR measured during the laboratory test. This test provides an estimation of the initial fire evolution in the Dalmarnock Test and the measured HRR is used as a first step towards the characterization of the ignition source. The main difference between the laboratory test and the actual Dalmarnock fire was that in the laboratory the heptane soaked blanket was not included. The HRR resulting from the burning blanket and the heptane was modelled following a fast t-square behaviour (see Fig. 2a) and then added to the experimental HRR. In addition to the fast fire assumption, the total energy released by the blanket is forced to match the energetic value according to Eq. (1):

\[
\int \text{HRR}_\text{blk} dt = m_{\text{blk}} \Delta h_{\text{c,blk}} + m_{\text{hep}} \Delta h_{\text{c,hep}},
\]

where \(m_{\text{blk}}\) is the initial mass of the blanket (estimated at 1.2 kg), \(h_{\text{c,blk}}\) its heat of combustion of cotton (16.5 MJ/kg [17]),
$m_{hep}$ is the mass of the heptane added to the blanket (0.07 kg for the estimated 100 ml poured over the blanket [5]) and $h_{c,hep}$ is the heat of combustion of heptane (44.5 MJ/kg [18]). A decay function of the form $(t - t_0)^2$ was introduced to complete the consumption of the blanket mass, where $t_0$ is the burnout time and set to 400 s. The resulting fast t-square fire for the blanket alone can be seen in Fig. 2a.

Camera footage of the Dalmarnock Test can be used to estimate the peak value of the HRR and support these approximations. The Dalmarnock fire spread quickly to the blanket and flames of about 1 m in length were observed at the location of the blanket. Using Heskestad's correlation, the HRR of a fire can be calculated from its size [19] as,

$$\dot{Q} = \left( \frac{L + 1.02D^\prime}{0.23} \right)^{5/2} L^{5/2}$$

where $\dot{Q}$ is the HRR, $L$ the flame length and $D^\prime$ the equivalent fire diameter. The blanket occupied an area with an equivalent diameter of 0.6 m. The HRR of a fire of this diameter corresponding to the observed 1 m high flames is of the order of 150 kW, in accordance with the peak HRR resulting from the fast t-square assumed here.

![Figure 2](image1.png)

**Figure 2:** a) Laboratory measured HRR of the basket and sofa fire, next to the approximated calculation for the blanket fire. b) Upper layer temperature during the growing phase (with blanket) comparing simulations and Dalmarnock measurements [5].

Using the combined measured and blanket HRR and applying it over the sofa area, the predicted average temperature of the upper layer in the room is in reasonable agreement with the measurement. A comparison between the simulated and measured is presented in Fig. 2b. The agreement last up to 200 s, then the simulated temperature decreases due to the predicted burnout of the basket and blanket fires and raises rapidly at 250 s when the bookshelf ignition and subsequent flashover is predicted (the raise is not shown in the figures). This dip was not observed in the Dalmarnock experiment. Thermocouples located between the basket and bookshelf next to the sofa at a height of 0.5 m show considerably higher temperatures (approx. 200°C higher) than those obtained in the simulations. This suggests that some fuel in the area was burning at that time, but there is no evidence to support this, since the area was not covered by CCTV cameras.

4.2. Fire location, fire area and heat of combustion

The total HRR is an important variable but the fire location and flame size and shape are as well important to predict the ignition of secondary objects and the growth phase. The diameter and height of the flame have a direct influence on the radiative heat fluxes to surrounding objects and on the air entrainment and thus on the convective heating of objects in the upper layer. For a given HRR, the pyrolyzate production rate per unit area affects the flame height by directly changing the buoyant strength of a fire and thus affecting air entrainment, burning rate and heating [11]. The varying HRR $\dot{Q}$ can be expressed as,

$$\dot{Q} = \Delta h_i \cdot A \cdot m_p,$$

where $\Delta h_i$ is the heat of combustion of the fuel, $A$ is the fire area, and $m_p$ is the pyrolyzate mass flow per unit area. For a fixed HRR, the mass flow increases either due to a decrease in the area or due to a decrease in the heat of combustion.

As seen in visual recordings during the growth phase of the Dalmarnock fire, the flames were not distributed over the entire sofa, but stayed predominantly in one third of the sofa near to the basket. Decreasing the fire diameter, but maintaining the imposed HRR, will then predict a higher flame according to Eq. 2. This increase in the flame height and the concentration of released heat on a smaller area changes the relationship between flame and surfaces from an optical point of view. Figure 3 shows the effect of changing the fire area (while keeping the HRR the same) on the upper layer temperature and the surface temperature of the nearby bookshelf. It is seen that the effect of the fire area is important on the surface temperature of the surrounding objects (Fig. 3b) while the effect is minor for the average temperature of the upper layer (Fig. 3a).

![Figure 3](image2.png)

**Figure 3:** Effect in the predictions of changing the fire area while keeping the HRR the same. a) average upper layer temperature with comparison to Dalmarnock measurements [5] b) bookshelf surface temperature of the bottom part of the bookshelf.

Given the importance of locating the origin of the HRR, the effect of separating the HRR measured in the laboratory between the basket and sofa portions and applying them in their respective locations was investigated. The decay from initial conditions to the growth inflection at 150 s seen in Fig. 2a is attributed to the burn out of the basket. If this HRR is deducted from the measurement what is left fits well a t-square fire of slow growth. This is attributed to the burning of the sofa alone. The basket HRR can be separated from the measurement and be distributed over a small area on the right side of the sofa representing the basket location. The blanket fire is added to the sofa fire and both are applied over an area of 1/3 of the sofa’s total.
horizontal surface. Figure 4 shows the effect of separating the HRR between the basket and the sofa on the upper layer temperature and the surface temperature of the nearby bookshelf. The separation of the two fires provides temperature predictions in the upper layer 20°C higher during the first 30 s, which is not a significant change. However, the difference is 40°C higher in the surface temperatures of the bookshelf which is important for the predictions of the ignition time of the bookshelf material. The significant effect of separating the basket fire is due to the small area of the basket and the relatively high HRR peak contributing to produce flames up to 1.3 m and so changing the geometry of the flame.

Another parameter that affects the flame height and the fire environment is the heat of combustion of the fuel, \( h_c \), used in the simulation. Decreasing the heat of combustion while keeping the HRR and the fire area fixed, results in an increase of the pyrolyzate mass flow per unit area (and vice versa), as expressed in Eq. 3. However, the Froude number, and thus the buoyant strength of the fire, is only affected weakly by the heat of combustion and thus a small effect is expected. The effect of changing this and also the fire area has been explored and the results are presented in Table 1 which shows the predicted flame heights for different sofa fire scenarios keeping the HRR fixed. The effect of changing the heat of combustion by more than 100% increases the predicted flame height by approx. 20-30%. Simulation with the lower heat of combustion shows that the change in the heat of combustion does not translate into a significant change in the time to ignition of the bookshelf.

4.3. Thermal and ignition material properties

The objects receiving incident heat flux from the fire will heat up according to their material properties [20]. In the Dalmarnock experiments, the bottom shelf of the bookshelf next to the sofa contained plastic boxes. Due to the small thickness of their walls the boxes can be considered as thermally thin, and therefore the parameter of interest for ignition predictions is the product of the thickness (\( \delta \)), density (\( \rho \)) and specific heat (\( c \)) [21]. The rate of change in the temperature of the object is proportional to the incident heat flux [21]:

\[
\rho c \frac{dT}{dt} = \dot{q}^{\text{net}}
\]  

where the net heat flux is the difference between the incident heat flux and the re-radiation:

\[
\dot{q}^{\text{net}} = \alpha \dot{q}'' - \sigma e T_w^4.
\]  

Table 1: Predicted flame heights on the sofa for different fires while keeping the HRR constant. Comparison with the observed values in the Dalmarnock Test One.

<table>
<thead>
<tr>
<th>Simulations</th>
<th>60 s flame height (m)</th>
<th>150 s flame height (m)</th>
<th>250 s flame height (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fire over entire sofa area</td>
<td>0.4</td>
<td>0.6</td>
<td>0.4</td>
</tr>
<tr>
<td>Fire over 1/3 sofa area</td>
<td>0.9</td>
<td>1.1</td>
<td>0.7</td>
</tr>
<tr>
<td>Fire over 1/3 sofa area and separated basket</td>
<td>0.8</td>
<td>1.1</td>
<td>0.6</td>
</tr>
<tr>
<td>Fire over 1/3 sofa area and lower ( h_b )</td>
<td>1.3</td>
<td>1.3</td>
<td>0.8</td>
</tr>
<tr>
<td>Observed in Dalmarnock</td>
<td>( \sim 1 )</td>
<td>( \sim 0.8 )</td>
<td>( \sim 0.8 )</td>
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</table>

Equation 4 can be integrated over time yielding the expression for the surface temperature as a function of time. The larger the thermal inertia \( \rho c \), the longer it takes for the surface to respond to the heating, and the peak temperature is not as high as it is for lower thermal inertias.

Figure 5 shows the surface temperature for different thermal inertias (\( \rho c \)). It shows that varying this parameter in 50% (from 1 to 0.5 kJ/m²/K) can produce important differences in the temperature of the surface (up to 40% between). Since the material properties of nearby objects or fuel packages are normally not known accurately, the sensitivity to this parameter is very important.

Figure 5: Effect of surface \( \rho c \) on the predicted bookshelf temperature at different heights a) 0.1 m above floor b) 1.5 m above floor.

Under Kirchhoff’s law [21], the emissivity of a surface represents the fraction of the total radiative power that the surface emits and absorbs. For relatively cold surfaces heated by a nearby fire, the absorption component dominates. Thus, this parameter has a double effect on the surface temperature, by establishing the fraction of incident radiation absorbed and the fraction re-radiated back into the gas phase.

A comparison of surface temperature for different emissivities is presented in Fig. 6. Near the flame, at 0.5 m above the
The heat feedback from the smoke is largely restricted to the upper layers but radiation of the compartment heat up the objects in the room. Convection from the smoke in the upper layers of the compartment heat up the objects in the room. Convective heating is largely restricted to the upper layers but radiation can heat up objects at lower layers. The heat feedback from the smoke layer might not be negligible and is investigated here in the context of the Dalmarnock fire.

In order to study the effect of the smoke layer on of the heating of surrounding objects, a simulation was conducted where the smoke easily escapes the compartment through a hole on the ceiling. This is not a realistic scenario but allows studying the case where all the smoke is removed. The predicted surface temperature is compared to the case where smoke accumulates. Figure 8 shows the surface temperature of the bookshelf at 0.5 and 1.5 m above the floor with smoke layer and without some layer. At 0.5 m, i.e. the height of the basket, there is no perceivable difference between both cases, whereas at 1.5 m above floor the temperatures differ approximately 10%. Since the bookshelf is tall and its upper parts are in direct contact with the hot smoke at 1.5 m, part of that difference can be attributed to convective heating from the smoke. It can be concluded that radiative heat feedback from the smoke layer during growth is not important in the Dalmarnock scenario for the ignition of objects outside the smoke layer, but that the convective part accounts for a significant increase in temperature of object within the smoke layer.

Considering that in FDS the radiation from the flame is modelled as a fraction of the HRR and thus it is decoupled from flame size and shape, it seems natural that soot production would not affect considerably the predicted incident heat flux. Figure 9 confirms this by showing that surface temperatures on the bookshelf do not vary in more than 7% while varying the soot yield produced in the combustion reaction in a range between 0.1 and 0.3.

5. Conclusions

It is widely accepted that the HRR is an essential variable in fire simulations. However, its value and evolution are rarely known beforehand in accidental fires. Then, the HRR must be estimated using fire dynamics, the lay-out of the scenario and material properties. When these parameters are studied, other parameters become also important in predicting fire dynamics. During the growth phase, the time to ignition of secondary items is important for predictions of fire spread and time to flashover. Radiation from the flame is to be one of the most important mechanisms for the ignition of nearby objects. The
location and area where the heat is released, and the height of the flame are important for flame radiation calculations. A smaller fire area and a higher pyrolyzate production rate for the same HRR will produce larger flame lengths.

The associated sensitivities of the upper layer temperature and surface temperature predictions have been quantified for the scenario of the large-scale Dalmarnock Test One. The results show that the global HRR in the compartment is a good input to predict the average temperatures in the compartment but produced poor prediction of the time to flashover. Simulations of the fire growth are significantly sensitive to the location of the HRR, fire area, material thermal properties, surface emissivity and flame radiative fraction, whereas the simulations are relatively insensitive to changes of the heat of combustion (while keeping the HRR constant), the soot yield and the heating from the smoke layer.

Since the material properties of nearby objects, surfaces and fuel packages are normally not known accurately, the sensitivity to this parameter is very important. Predictions of secondary ignition, fire spread and thus of time to flashover can depend strongly on the appropriate estimation of these material and fire parameters.

The development of fire forecasting methodologies in support of the emergency response must focus on the variables identified here as important. The live sensor data could be used to update and provide some sort of best estimates of these parameters and to reduce the associated uncertainty. These parameters then could be used in the computational predictions. Since heat feedback from the smoke layer during fire growth is not significant for objects outside the smoke layer, the results here suggest that for predictions of secondary ignition and flashover, fire CFD modelling may not be justified in terms of accuracy, and other, simpler and computationally cheaper models could be used to accelerate computational fire forecasts.

References


