Recent Advancement of Soot Prediction in Fire Field Model with the Incorporation of Detailed Combustion Products for Compartment Fires

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ABSTRACT

In compartment fires, soot is an inevitable factor since it forms during incomplete combustion which consumes energy while aggregates at the ceiling. Soot particulates can act as a radiative heat transfer medium which may affect the fire development drastically. Correspondingly, when performing fire simulations using fire field models, it is essential to implement a soot model which considers the formation processes of soot particles. There are several key elementary chemical processes which may result in the generation or reduction of the number or size of soot particles including: nucleation, coagulation, surface growth, agglomeration and oxidation. In particularly, it is believed by many researchers that acetylene \( \text{C}_2\text{H}_2 \) plays an important role to the formation processes of soot as it is the main hydrocarbon by-product that contributes to the generation of aromatics. Furthermore, hydroxyl radiacal is the major oxidizer for the oxidation process of soot particles. In this study, a fire field model based on large eddy simulation (LES) approach has been developed which incorporates detailed chemical kinetics for combustion, as well as other essential fire modelling components. With a comprehensive description of the fuel oxidation processes as well as formation of hydrocarbons, the concentration of \( \text{C}_2\text{H}_2 \) and \( \text{OH} \) can be correctly simulated in the model. Therefore, the inclusion of detailed chemical products also enhances the modelling of soot particles. The Moss-Brookes two equation semi-empirical soot model is thereby utilized in the code. It considers the concentration of \( \text{C}_2\text{H}_2 \) as the main precursor for the reaction rates of the soot formation processes while taking \( \text{OH} \) as the oxidizer for soot oxidation. In general, the simulation showed an averaged improvement of 31.69% in the prediction of soot particle volume fraction.

KEYWORDS: Combustion, fire simulation, large eddy simulation, soot.

NOMENCLATURE

- \( C_A \): Moss model contant for nucleation \( (\text{m}^3 \cdot \text{kg}^{-2} \cdot \text{K}^{-1/2} \cdot \text{s}^{-1}) \)
- \( C_B \): Moss model contant for coagulation \( (\text{m}^3 \cdot \text{K}^{-1/2} \cdot \text{s}^{-1}) \)
- \( C_Y \): Moss model contant for surface growth \( (\text{kg}^{-2/3} \cdot \text{K}^{-1/2} \cdot \text{s}^{-1}) \)
- \( C_\alpha \): Moss-Brookes model contant for nucleation \( (\text{s}^{-1}) \)
- \( C_\beta \): Moss-Brookes model contant for coagulation \( (\text{s}^{-1}) \)
- \( C_\gamma \): Moss-Brookes model contant for surface growth \( (\text{kg} \cdot \text{m} \cdot \text{kmol}^{-1} \cdot \text{s}^{-1}) \)
- \( f_v \): soot volume fraction \((-)\)
- \( M \): molecular weight \( (\text{g} \cdot \text{mol}^{-1}) \)
- \( n \): soot number density \((-)\)
- \( N \): alternative soot number density \((-)\)
- \( N_0 \): Avogadro constant \( (\text{mol}^{-1}) \)
- \( T \): temperature \( (\text{K}) \)
- \( t \): time \( (\text{s}) \)
**INTRODUCTION**

In actual building fires, smoke inhalation is arguably the main hazard that causes human deaths or serious injuries including lung damages. Therefore, one of the key and challenging aspects in compartment fire simulation is to model the generation and movement of smoke. Soot particles (i.e. mainly composed of carbon) are the visible airborne solid contaminant that produces the black/grey colour in the cloud of smoke. According to Drysdale [1], soot particles are formed during incomplete combustion and pyrolysis under limited oxygen and high temperature conditions. Recently, with the advancement achieved in combustion modelling, more research efforts have been carried out on the modelling on soot formation and oxidation processes.

One of the earliest soot formation model was proposed by Tesner et al. [2]. In their model, the soot formation process was separated into two phases. The first step described the formation of soot radical nuclei and the second step depicted the growth of soot particles from the branching of nuclei. Later, Tesner’s model was extended by Magnusen and Hjertager [3] with the application of the eddy dissipation concept. Another alternative model was developed by Khan et al. [4] which has been widely adopted for numerical study on diesel engines. Luo and Beck [5] applied Tesner’s model on the simulation of a full-scale multiple compartment room to simulate the temperature development during flashover and reasonable comparisons with experiment data were achieved.

Later, soot models based on two transport equations were proposed including the developments by Moss et al. [6], Syed et al. [7], Leung et al. [8] and Brookes and Moss [9]. These models incorporate the physical process of soot formation: soot nucleation, coagulation and surface growth which will be discussed in more detail in Chapter 8. In the transport equations, the soot volume fraction and number density of particles are considered. The performance of Moss’s model was investigated in the compartment fire study conducted by Cheung et al. [10]. The model was compared with Khan’s and Tesner’s models while Moss’s model produced the most accurate temperature predictions against the experiment.

Models that describe the detailed elementary chemical reactions and physics of soot formation can be subsequently applied if the detailed chemistry of these parent fuels is known. Frenklach and Wang [11] proposed a detailed kinetic models for the gas-phase phenomena for hydrocarbon fuels to describe the successive chemical steps and the presence of pyrolysis products such as acetylene, which are generally considered as critical participating species in the nucleation process. Nonetheless, there is a need to formulate reduced chemical mechanisms to predict the consumption of heavy hydrocarbons. Moreover, there is a greater requirement in field modelling to gain further insights into the combustion chemistry of complex fuels, which was explored extensively in this study.
NUMERICAL MODELLING

A three-dimensional numerical model using large eddy simulation (LES) approach has been developed specifically for in-house fire simulations. The code is able to simulate the temporal turbulent reacting fire behaviour for compartment fire scenarios and has been validated in previous studies [12-14]. It is associated with sub-modelling components including the Wall-Adapting Local Eddy Viscosity (WALE) subgrid-scale (SGS) turbulence model, the presumed probability density function (PrePDF) combustion model, as well as the discrete ordinates method (DOM) radiation model. The GRI-Mech 3.0 proposed by the Gas Research Institute (GRI), US which comprises the complete set of elementary chemical reactions containing 325 reactions and 53 species, is adopted in the commercial software CHEMKIN 3.6 to generate the flamelet profiles used in the PrePDF combustion model. Since this article focus on the modelling of the soot generation, the formulations for the aforementioned models are detailed in past publications [13].

Soot formation and destruction is a complex phenomenon as the size of soot particles can vary between wide ranges. In semi-empirical models, a conserved property known as the “number density” was introduced to represent the degree of concentration of the particle size group. As a result, the quantity of soot particles are now indicated by two conserved properties including the soot mass fraction or soot volume fraction along with the soot particulate number density, which are resolved by two transport equations. The objective of the semi-empirical models is to incorporate some level of physics and chemistry of the soot formation mechanisms. Most of these models comprise four major soot formation processes including nucleation, surface growth, coagulation and oxidation, which are generally represented in the form of reaction rate equations of soot precursors and particles with chemical description. In this study, two semi-empirical models for soot formation were adopted on the predictions of soot particles in compartment fires.

Moss model

The first semi-empirical model employed in this study was developed by Moss et al. [6]. The properties of soot are represented by two conservative variables – soot volume fraction, \( f_v \), and the particulate number density or radical nuclei, \( n \). The transport equations are balanced based on simplified descriptions of the processes of nucleation, surface growth and coagulation involved in soot formation in non-premixed flames. The transport equations for the filtered soot volume fraction \( \tilde{v}_{\text{soot}} \) and the filtered soot particulate number density \( \tilde{n}_{\text{soot}} \) are expressed as:

\[
\frac{\partial (\tilde{p} \tilde{v}_{\text{soot}})}{\partial t} + \frac{\partial (\tilde{p} \tilde{u}_i \tilde{v}_{\text{soot}})}{\partial x_i} = - \frac{\partial (\tilde{p} \tilde{u}_i \tilde{v}_{\text{soot}})}{\partial x_i} + \frac{\partial}{\partial x_i} \left( \frac{\mu_f}{Sc_f} \tilde{v}_{\text{soot}} \right) + \tilde{S}_{\text{soot}}, \quad (1)
\]

\[
\frac{\partial (\tilde{p} \tilde{n}_{\text{soot}})}{\partial t} + \frac{\partial (\tilde{p} \tilde{u}_i \tilde{n}_{\text{soot}})}{\partial x_i} = - \frac{\partial (\tilde{p} \tilde{u}_i \tilde{n}_{\text{soot}})}{\partial x_i} + \frac{\partial}{\partial x_i} \left( \frac{\mu_f}{Sc_f} \tilde{n}_{\text{soot}} \right) + \tilde{S}_{\text{n,soot}}, \quad (2)
\]

where the variables \( \tilde{v}_{\text{soot}} \) and \( \tilde{n}_{\text{soot}} \) are alternative definitions of soot volume fraction and particulate number density given as \( \tilde{v}_{\text{soot}} = \rho_{\text{soot}} f_v / \tilde{p} \) and \( \tilde{n}_{\text{soot}} = \tilde{n}_{\text{soot}} / (\tilde{p} N_0) \) respectively, in which \( \rho_{\text{soot}} \) is the mass density of soot and \( N_0 \) is the Avogadro number. In the transport equations, the mean thermophoretic velocity component \( U_{th} \) is provided as \(-0.54(\mu / \tilde{p}) \partial / \partial x_i \ln(\tilde{T})\). The source terms for soot volume fraction and particulate number density are expressed as:
Part II Fire

\[ \tilde{S}_{N,\text{soot}} = \tilde{\alpha} - \tilde{\beta}^2 \tilde{\eta}_{\text{soot}}^2, \]  
(3)

\[ \tilde{S}_{V,\text{soot}} = \tilde{\delta} - N_0^{1/3} \tilde{\rho} \tilde{\eta}_{\text{soot}}^{2/3} \tilde{\eta}_{\text{soot}}^{-1/3}, \]  
(4)

where the filtered term \( \tilde{\alpha} \) in Eq. (3) depicts the increase in number density of soot particle caused by particle nucleation or inception, and the other filtered term \( \tilde{\beta} \) represents the reduction of soot particulate number density due to coagulation of particles. The particle inception rate \( \tilde{\alpha} \) can be calculated as reaction rate equation with the concentration of fuel as the precursor, whereas the coagulation term \( \tilde{\beta} \) is evaluated based on the Smoluchowski’s expression [15], which are given as:

\[ \tilde{\alpha} = C_A \tilde{\rho} \tilde{T}^{1/2} \tilde{X}_f \exp \left( -\frac{T_A}{\tilde{T}} \right), \]  
(5)

\[ \tilde{\beta} = C_B \tilde{T}^{1/2}. \]  
(6)

For the balance of soot volume fraction, the filtered terms \( \tilde{\delta} \) and \( \tilde{\tau} \) in Eq. (4) describe the growth in soot volume fraction produced by nucleation of particles and surface growth respectively. According to the particle inception rate \( \tilde{\alpha} \) introduced in the number density source term expression, the rate of nucleation for soot volume fraction is based on the consideration of the molecular mass of 12 carbon atoms given by:

\[ \tilde{\delta} = M_{p,\text{soot}} \tilde{\alpha}, \]  
(7)

where \( M_{p,\text{soot}} \) is the mass of an incipient soot particle (i.e. taken as the molecular mass of 12 carbon atoms hence \( M_{p,\text{soot}} = 144 \text{ kg} \cdot \text{kmol}^{-1} \)). The expression of the surface growth rate is suggested by Syed et al. [7], which contains a linear dependence on aerosol surface area and is provided as a reaction rate expression in term of fuel concentration as:

\[ \tilde{\tau} = C_f \tilde{\rho} \tilde{T}^{1/2} \tilde{X}_f \exp \left( -\frac{T_f}{\tilde{T}} \right), \]  
(8)

where the pre-exponential constants \( C_A, C_B, C_f \) and the activation temperatures \( T_A, T_f \) appeared in the above equations are summarised in Table 1.

**Table 1.** Pre-exponential constants for soot nucleation, surface growth and coagulation rate equations for the Moss model.

<table>
<thead>
<tr>
<th>Constants</th>
<th>Empirical values</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>( C_A )</td>
<td>65400</td>
<td>( \text{m}^3 \cdot \text{kg}^{-2} \cdot \text{K}^{-1/2} \cdot \text{s}^{-1} )</td>
</tr>
<tr>
<td>( C_B )</td>
<td>( 1.3 \times 10^7 )</td>
<td>( \text{m}^3 \cdot \text{K}^{-1/2} \cdot \text{s}^{-1} )</td>
</tr>
<tr>
<td>( C_f )</td>
<td>0.1</td>
<td>( \text{kg}^{-2/3} \cdot \text{K}^{-1/2} \cdot \text{s}^{-1} )</td>
</tr>
<tr>
<td>( T_A )</td>
<td>46100</td>
<td>K</td>
</tr>
<tr>
<td>( T_f )</td>
<td>12600</td>
<td>K</td>
</tr>
</tbody>
</table>

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Moss-Brookes model

The second semi-empirical model utilised in this study was proposed by Brookes and Moss [9]. It incorporates the essential physical processes of soot particle inception, coagulation, surface growth and oxidation. Similar to the Moss model, this approach consists of two transport equations, but the mass fraction of soot is taken in conjunction with the number density of soot particles as the define conserved properties, which are expressed as:

\[
\frac{\partial \left( \rho \tilde{Y}_{\text{soot}} \right)}{\partial t} + \frac{\partial \left( \rho \tilde{u}_i \tilde{Y}_{\text{soot}} \right)}{\partial x_i} = - \frac{\partial \left( \rho \tilde{u}_{i \text{th}} \tilde{Y}_{\text{soot}} \right)}{\partial x_i} + \frac{\partial \left( \rho u_i \tilde{Y}_{\text{soot}} \right)}{\partial x_i} + \frac{\partial }{\partial x_i} \left( \frac{\mu_f}{Sc_f} \frac{\partial \tilde{Y}_{\text{soot}}}{\partial x_i} \right) + \tilde{S}_{Y,\text{soot}} , \tag{9}
\]

\[
\frac{\partial \left( \rho \tilde{N}_{\text{soot}} \right)}{\partial t} + \frac{\partial \left( \rho \tilde{u}_i \tilde{N}_{\text{soot}} \right)}{\partial x_i} = - \frac{\partial \left( \rho \tilde{u}_{i \text{th}} \tilde{N}_{\text{soot}} \right)}{\partial x_i} + \frac{\partial \left( \rho u_i \tilde{N}_{\text{soot}} \right)}{\partial x_i} + \frac{\partial }{\partial x_i} \left( \frac{\mu_f}{Sc_f} \frac{\partial \tilde{N}_{\text{soot}}}{\partial x_i} \right) + \tilde{S}_{N,\text{soot}} , \tag{10}
\]

where the source terms in Eq. (9) and Eq. (10) are given as:

\[
\tilde{S}_{N,\text{soot}} = \alpha - \beta , \tag{11}
\]

\[
\tilde{S}_{Y,\text{soot}} = \delta + \gamma - \zeta , \tag{12}
\]

where the above source terms \( \tilde{S}_{N,\text{soot}} \) and \( \tilde{S}_{Y,\text{soot}} \) represent the instantaneous production rate of soot particles and the rate of increase in number density of particles respectively, in which \( \tilde{S}_{N,\text{soot}} \) is calculated by the reaction rates \( \alpha \) and \( \beta \) given as:

\[
\alpha = C_\alpha N_0 \left( \frac{X_{C_2H_5}}{RT} \right)^2 \exp \left( - \frac{T_a}{\tilde{T}} \right) , \tag{13}
\]

\[
\beta = C_\beta \left( \frac{24 \times RT}{P_{\text{soot}} N_0} \right)^{1/2} d_p^{1/2} \tilde{N}^2 . \tag{14}
\]

It should be addressed that the modelling constants \( C_\alpha \) and \( C_\beta \) are not the same as the ones for the Moss model, since the solution algorithm for the reaction rates are different in the Moss Brookes model. The filtered terms \( \tilde{\alpha} \) and \( \tilde{\beta} \) describes the soot particle generation rates due to particle inception and coagulation respectively. On the other hand, the reactions rates filtered terms \( \tilde{\delta} \), \( \tilde{\gamma} \) and \( \tilde{\zeta} \) in Eq. (12) represents the increase rate of number density caused by the processes of particle nucleation and surface growth, and reduction rate owing to oxidation, which are evaluated as:

\[
\tilde{\delta} = M_{\beta,\text{soot}} \tilde{\alpha} , \tag{15}
\]

\[
\tilde{\gamma} = C_\gamma \left( \frac{X_{C_2H_5}}{RT} \right)^{1/4} \exp \left( - \frac{T_a}{\tilde{T}} \right) \left( \pi \tilde{N} \right)^{1/3} \left( \frac{6 \tilde{Y}_{\text{soot}}}{P_{\text{soot}}} \right)^{2/3} , \tag{16}
\]

\[
\tilde{\zeta} = C_\omega C_{\text{oxid}} T_{\text{coll}} \left( \frac{X_{\text{OH}}}{RT} \right) \sqrt{\tilde{T}} \left( \pi \tilde{N} \right)^{1/3} \left( \frac{6 \tilde{Y}_{\text{soot}}}{P_{\text{soot}}} \right)^{2/3} , \tag{17}
\]
where the filtered nucleation rate also described by the mass of an incipient soot particle $M_{\text{p,soot}}$ taken as $144 \text{ kg} \cdot \text{kmol}^{-1}$. $C_{\text{oxid}}$ is the oxidation rate scaling parameter and $\eta_{\text{coll}}$ is the collisional efficiency parameter can be given as 0.015 and 0.04 respectively suggested by Puri et al. [17]. According to empirical correlations reported by Brookes and Moss [9], the pre-exponential constants $C_{\alpha}$, $C_{\beta}$, $C_{\gamma}$, $C_{\zeta}$ and activation temperatures $T_{\alpha}$, $T_{\gamma}$ in Eq. (15) to Eq. (17) are summarised Table 2.

**Table 2.** Pre-exponential constants for soot nucleation, surface growth and coagulation rate equations for the Moss Brookes model.

<table>
<thead>
<tr>
<th>Constants</th>
<th>Empirical values</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{\alpha}$</td>
<td>54</td>
<td>$\text{s}^{-1}$</td>
</tr>
<tr>
<td>$C_{\beta}$</td>
<td>1</td>
<td>$\text{s}^{-1}$</td>
</tr>
<tr>
<td>$C_{\gamma}$</td>
<td>430</td>
<td>$\text{kg} \cdot \text{m} \cdot \text{kmol}^{-1} \cdot \text{s}^{-1}$</td>
</tr>
<tr>
<td>$C_{\zeta}$</td>
<td>105.8125</td>
<td>$\text{kg} \cdot \text{m} \cdot \text{kmol}^{-1} \cdot \text{K}^{-1/2} \cdot \text{s}^{-1}$</td>
</tr>
<tr>
<td>$T_{\alpha}$</td>
<td>21000</td>
<td>$\text{K}$</td>
</tr>
<tr>
<td>$T_{\gamma}$</td>
<td>12100</td>
<td>$\text{K}$</td>
</tr>
</tbody>
</table>

**NUMERICAL CASE STUDY**

In order to examine the effectiveness of the code in the simulation of soot production, numerical simulations have been performed on a 2/5 reduced-scale ISO compartment room experiment carried out by the National Institute of Standard and Technology (NIST), US. This experiment was provided with gas sampling systems and soot probe measurements. The size of the 2/5 reduced-scale ISO compartment room are $1.42 \text{ m} \times 0.95 \text{ m} \times 0.98 \text{ m}$ (i.e. length $\times$ width $\times$ height). A $0.13 \text{ m} \times 0.13 \text{ m}$ square gravel-filed burner with natural gas fuel was placed at the centre of the room and it is raised 0.15 m above the ground. Compartment walls were constructed by two layers of 1.27 cm thick calcium silicate boards (Marinite I) for insulation purpose. The burn room was raised by 0.2 m during the experiment. Locations for the measurements were reported in detail by Bryner et al.[17].

Fig. 1 shows the computational domain for the numerical model. It should be noted that the compartment room was placed within an extended physical volume of $3 \text{ m} \times 2.95 \text{ m} \times 3.2 \text{ m}$. This is owing to the fact that the extended region provided improved predictions for flow and energy at the doorway opening. In essence, the air movement outside the compartment room was modelled before entering the compartment, hence providing a more realistic incoming and outgoing flow profile at the opening.
RESULTS AND DISCUSSIONS

Two simulation settings have been performed during numerical assessment. Firstly, the Moss model was associated with multi-step reaction scheme chemistry for combustion; secondly, the Moss-Brookes model was associated with detailed chemistry for combustion. This is due to the fact that the Moss-Brookes model requires the prediction of acetylene in order to operate, which is included in detailed chemistry. In this section, the two simulation cases are represented by the short form “MM” and “DMB” referring to “Moss” and “Moss-Brookes” respectively. Furthermore, four heat release rates were considered for comparisons with experimental results including 74 kW, 116 kW, 265 kW and 408 kW.

Soot concentration predictions

Since the flame is deflected towards the opening, fuel is richer at the front portion of the compartment. For the multi-step scheme, soot is directly dependent to the composition of fuel mass within the mixture. For the detailed scheme, as hydrocarbon products including the soot precursor acetylene C$_2$H$_2$ are formed by fuel oxidation processes, the formation of soot particles also occurs at the front compartment region. Consequently, the content of soot particles predicted at the front sample probe is found to be higher than the rear sample probe in both simulation Cases MM and DMB as indicated in Table 3 respectively. It should be noted that there was a large anomaly of measured data observed for 408 kW at the front sample probe which could be due to instrumental error, thus this result is not demonstrated in this paper. By considering C$_2$H$_2$ as the parent incipient rather than the fuel itself, it is clearly shown that level of soot particles approximated in Case DMB is significantly less than Case MM, which are in better agreement with the measured value analysed by the soot sampling system. On the other hand, the concentrations of soot particles are greatly over-estimated by the Moss model, indicating that fuel is not an appropriate precursor for the soot models. Although improvements are achieved by applying the Moss-Brookes model, some deviations against the experimental data are observed especially for low fire sizes. It is postulated that a more comprehensive SGS soot formation model that describes the full reaction processes can further improve the numerical results. An averaged relative difference of 10.9% was recorded by Case DMB against experimental data (i.e. excluding the front probe data for 408 kW), which gives
an average improvement of 37.11% and 27.63% over Case MM at the front and rear probes respectively.

Table 3. Soot concentration comparisons between numerical and experimental results at the front probe.

<table>
<thead>
<tr>
<th>Heat release rate (kW)</th>
<th>Experiment (kW) ±0.01</th>
<th>Numerical (MM)</th>
<th>% error (MM)</th>
<th>Numerical (DMB)</th>
<th>% error (DMB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>74</td>
<td>0.01 ±0.01</td>
<td>0.1917</td>
<td>94.78</td>
<td>0.03407</td>
<td>77.31</td>
</tr>
<tr>
<td>179</td>
<td>0.09 ±0.01</td>
<td>0.2375</td>
<td>62.11</td>
<td>0.1035</td>
<td>13.04</td>
</tr>
<tr>
<td>265</td>
<td>0.17 ±0.01</td>
<td>0.2919</td>
<td>41.76</td>
<td>0.1650</td>
<td>3.03</td>
</tr>
</tbody>
</table>

Table 4. Soot concentration comparisons between numerical and experimental results at the rear probe.

<table>
<thead>
<tr>
<th>Heat release rate (kW)</th>
<th>Experiment (kW) ±0.01</th>
<th>Numerical (MM)</th>
<th>% error (MM)</th>
<th>Numerical (DMB)</th>
<th>% error (DMB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>74</td>
<td>0.01 ±0.01</td>
<td>0.1151</td>
<td>91.31</td>
<td>0.05218</td>
<td>80.83</td>
</tr>
<tr>
<td>179</td>
<td>0.08 ±0.01</td>
<td>0.1743</td>
<td>54.10</td>
<td>0.1085</td>
<td>26.27</td>
</tr>
<tr>
<td>265</td>
<td>0.15 ±0.01</td>
<td>0.2426</td>
<td>38.17</td>
<td>0.1450</td>
<td>3.45</td>
</tr>
<tr>
<td>408</td>
<td>0.17 ±0.01</td>
<td>0.3075</td>
<td>44.72</td>
<td>0.1980</td>
<td>14.14</td>
</tr>
</tbody>
</table>

Carbon monoxide/dioxide and soot contour plots

The contents of combustion products within the ISO room for the 74 kW fire for Case DMB are represented by the CO$_2$ and CO contour plots in Fig. 2(a) and Fig. 2(b) respectively. It can be observed that the concentration of CO$_2$ is the richest at the upper compartment region. On the contrary, the majority of the concentration of CO is contained within the flame region. The incipient for soot particles, C$_2$H$_2$ is mainly generated at the core of the flame as illustrated in Fig. 2(c). This is reasonable since C$_2$H$_2$ is formed by reactions between fuel and other hydrocarbon compounds which majorly exists within the flame zone. Considerable amount of soot particles are generated and contained near the ceiling of the compartment as depicted in Fig. 2(d).
CONCLUSIONS

An in-house three dimensional LES based numerical model specifically for fire simulations has been developed. It considers the detailed chemical kinetics for the soot formation process and combustion. Numerical simulations were performed on a 2/5 ISO room experiments with comprehensive soot probe measurements to examine the accuracy of the Moss-Brookes semi-empirical soot model with detailed chemistry against the Moss model with multi-step reaction scheme. The comparisons with the soot sampling data suggest that Moss-Brookes model is more capable of predicting the soot particle field over Moss model with an overall average improvement of 31.69% in terms of percentage error. Since Moss-Brookes model considers acetylene as the soot precursor while Moss model considers the fuel as precursor, the Moss-Brookes model provides a better representation of the nucleation, surface growth and oxidation processes of soot particles.

REFERENCES