Application of a subgrid soot-radiation model in the numerical simulation of a heptane pool fire

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Abstract

Predictions of temperature, soot volume fraction and incident radiant flux are presented from large-eddy simulations of a medium-scale heptane pool fire. A subgrid soot-radiation model, which is based on the laminar smoke point concept, is applied to provide local emission from the turbulent flame-sheet. A local absorption coefficient is estimated using the local emission, mesh resolved temperature and its modeled subgrid variance. Absorption–emission calculations are conducted with the solution of the radiative transport equation (RTE). The results obtained from the fire simulations including velocity, temperature, volumetric emission and soot concentration distributions are compared with general observations from the experiment. Radial profiles of temperature and soot volume fraction are also compared with experimental data at several heights above the burner. Predicted temperature profiles are found to generally agree with the experimental data. Soot volume fraction predictions show similar trends as experimental measurements with positive and negative deviations. Incident radiation at an axial location away from the fire shows good agreement between the model and the experiment.

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1. Introduction

Pool fires can result from ignition of accidental spills of ignitable liquids. These fires involve high heat release rates and, in cases where sooty fuels are present, high radiant emissions that can result in the spread of fire to neighboring objects. Recent reviews have discussed both the turbulent fluid mechanics of fires [1] and the role of radiation heat transfer in fire phenomena [2]. Both the turbulent burning process and its interaction with radiation are important phenomena in predictions of heat transfer phenomena in pool fires.

Recent pool fire radiation studies have extracted curve fits of experimental data to generate time averaged two- and three-dimensional spatial distributions of temperature, species and soot [3,4]. Avoiding the solution of unsteady Navier–Stokes equations provided the studies the opportunity to apply detailed models for radiation heat transfer,
In LES a substantial fraction of energy remains in the subgrid and in buoyant flows associated with fires the subgrid energy is evidently anisotropic in character. Therefore, transport of the subgrid kinetic energy is included for turbulence closure. The SGS turbulent viscosity, \( \nu_s \), in the momentum equations is computed from the solution of \( k_{sgs} \) as described in Fureby et al. [12]. The dissipation of \( k_{sgs} \) is modeled as \( \varepsilon_{sgs} = c_{e,sgs} k_{sgs}^{3/2} \Delta^{-1} \) [12]. The constant \( c_e \) is equal to 1.048 and \( \Delta \) is the LES filter size [12]. The turbulent viscosity is computed as \( \nu_t = c_t \Delta^{1/2} \). The constant \( c_t \) is estimated from a localized dynamic procedure following the application of a test filter [13]. The localized dynamic procedure produces a distribution of \( c_t \) as an attempt to capture the influence from the anisotropic scales of turbulence present in different parts of the fire.

2.2. Radiation modeling

2.2.1. Flamelet model for soot-emission

The flamelet model postulates a 1-D transient packet of fuel being stretched by a constant strain rate normal to its axis [7]. The model applies the laminar smoke-point concept [14] to describe soot formation, oxidation and radiation. As in previous studies [7,15], the flamelet calculations use an absorption coefficient computed as \( \kappa = \kappa_s + \kappa_g \approx \kappa_S \), where \( \kappa_S \) is assumed to include soot (\( \kappa_s \)) and gas-phase (\( \kappa_g \)) contributions. The equivalent \( \kappa_S \) is estimated with the application of the laminar smoke point model [14]. Such an approximation can be justified when radiation from fires is dominated by soot-radiation as in toluene, heptane and ethylene fires [8,16].

The flamelet model [7] provides the local radiant emission fraction, \( \Psi_r \), of the turbulent flame-sheet taking two inputs from the LES solver, the non-dimensional prior heat loss/gain, \( H_p \), and the micro-scale strain rate, \( a_0 \), and returns the local volumetric radiant emission term, \( \dot{q}_r^m = \Psi_r (H_p, a_0) \dot{\omega}_r^m \Delta H_c \), where \( \dot{\omega}_r^m \) is computed from the EDM model [11] and \( \Delta H_c \) is the fuel heat of combustion. The characteristic strain rate, \( a_0 \), is estimated as the inverse of the Kolmogorov micro-time, \( a_0 = C_\eta \tau_k^{-1} \). Based on previous studies [15] involving constant \( c_k \) values used in turbulence modeling, \( C_\eta \) was found to depend inversely on the selection of \( c_k \) values. This was because the choice of \( c_k \) influenced the prediction of strain rates in the fires. This relationship, \( C_\eta \approx 1/c_k \), is preserved in the present simulations where \( c_k \) is spatially varying. Radiant emission from the flamelet increases with reducing strain rate and prior loss, with peak values occurring for prior heat gain. A prior heat gain is possible in the fire when cold soot absorbs incoming radiation resulting in an increase in the enthalpy of the grid cell.
2.2.2. Absorption coefficient estimation

The optically-thin emission model [7] summarized above is developed to include the effect of absorption (due to soot) on flame radiation. The volumetric emission, $\tilde{q}_v^m$, is used along with an estimate of a mean flame-sheet temperature in a computational cell to estimate the local absorption coefficient, $\tilde{\kappa}$, required for the absorption–emission calculations. The primary issue with estimation of $\tilde{\kappa}$ from $\tilde{q}_v^m$ is the difficulty in estimation of mean flame-sheet temperature, primarily because the flame-sheet is not resolved in LES of diffusion flames. TRI correlations and modeled subgrid temperature variance are applied for mean flame-sheet temperature estimation, as described below.

For a gray media assumption, the divergence of the radiative heat flux is written as

$$\nabla \cdot \text{q}_v = 4\sigma \kappa \tilde{I}^4 - \kappa \tilde{G},$$

where, the emission term, $4\sigma \kappa \tilde{I}^4$, is equivalent to $\tilde{q}_v^m$, which is a known quantity as described above. The emission term can be expanded, similar to the expansion by Sneigirev [17], providing temperature self-correlation and a correlation between the filtered absorption coefficient and temperature,

$$\kappa \tilde{I}^4 = \tilde{\kappa} \tilde{I}^4 \left( \frac{T_i^4}{T_i^4} + \frac{\kappa_i \tilde{I}^4}{\tilde{\kappa} \tilde{I}^4} \right) = \tilde{\kappa} \tilde{I}^4 (R_{j}^4 + R_{i}^4). \tag{1}$$

The correlation $R_{j}^4$ is estimated by expanding it and dropping higher than second order terms and with the assumption that $\tilde{I}^4 = 0$, as $R_{j}^4 \approx 1 + 6C_{\text{TRI}} \tilde{I}^4 / \tilde{I}^4$. The constant $C_{\text{TRI}}$ accounts for the contribution of the neglected higher-order terms [17]. Previous studies [17,18] have established the importance of the $R_{j}^4$ correlation which represents the dominant phenomenon in TRI due to the strong non-linear dependence of emissive power on temperature [17,19]. In contrast, the $R_{i}^4$ term in Eq. (1), which can be approximated as $R_{i}^4 \sim \partial \kappa / \partial T_T^4 \tilde{I}^4 / (\tilde{\kappa} \tilde{I}^4)$, is expected to have a small magnitude. It is also difficult to estimate the derivative $\partial \kappa / \partial T_T$ for gas-soot mixtures. Therefore, in the present study, $R_{i}^4$ is neglected and $R_{j}^4$ only is included as a first estimate of TRI on radiation calculations. The absorption coefficient, $\tilde{\kappa}$, is estimated by equating the emission occurring at a mean turbulent flame-sheet temperature, i.e. $T_{j}^4 \approx \tilde{I}^4 (1 + 6C_{\text{TRI}} \tilde{I}^4 / \tilde{I}^4)$. In Eq. (2), the $T_{j}^4$, $\tilde{T}$, and the radiant emission, $\tilde{q}_v^m$, are obtained from the LES solver, whereas the variance of temperature is modeled as $\tilde{T}^4 \sim \Delta^3 |\nabla T|^3$. From Eq. (2), the soot volume fraction, $f_s$, can be computed, assuming there is a weak correlation between the unresolved components of soot volume fraction and temperature, i.e. $f_s T = \tilde{f}_s \tilde{T} + f_s^0 \tilde{I}^4 \approx \tilde{f}_s \tilde{T}$ [17,19], as $f_s \approx \kappa / [3.83(C_0/C_2) \tilde{T}]$, where $C_0 = 5.58$ and $C_2$ is Planck’s second constant [8,20].

In order to perform absorption–emission calculations the approximation $\kappa \tilde{G} \approx \tilde{\kappa} \tilde{G}$ is made, which assumes the correlation between absorption coefficient and intensity is weak, i.e. absorption TRI is neglected. This assumption is known as the optically transparent fluctuation assumption (OTFA) [18]. Different studies have concluded in favor of including the absorption TRI [21] or omitting it for simplicity [22]. The OTFA assumption holds well for optically intermediate scenarios whereas the assumption may fail when heavily sooting fuels (e.g. toluene) are involved, making self-absorption modeling in turbulent eddies a necessity. The divergence of the radiative heat flux in the present study is then computed from the solution of the RTE as $\nabla \cdot \text{q}_v = \tilde{q}_v^m - \tilde{\kappa} \tilde{G}$, where, the absorption coefficient, $\tilde{\kappa}$, is computed from Eq. (2).

2.2.3. RTE solution

The finite volume method (FVM) available in OpenFOAM [10] is used for solution of the RTE with angular discretization involving 48 solid angles ($N_\phi = 12 \times N_\theta = 4$). The selected angular discretization was found to be adequate for radiative exchange inside the fire, however a higher total number of angles ($N_\phi = 12 \times N_\theta = 8$) was needed to provide distributions of incident radiant heat flux comparable to experimental measurements at an axial distance of 0.825 m.

2.3. Computational setup

The computational setup shown in Fig. 1 consisted of a 0.3 m diameter circular burner elevated...
from the ground by 0.15 m. The overall domain was of circular cross section with a diameter of 0.825 m and height of 3.9 m. The mesh was comprised primarily of hexahedral cells. Based on a mesh sensitivity study, a mesh resolution of \((0.008 \text{ m})^3\) was determined as providing converged results. Results were time-averaged for 120 s avoiding the results from an initial transient of \(\sim 60\) s.

The side boundaries were open allowing entrainment of air whereas the ground and burner side had a slip boundary condition applied for velocity. The slip boundary condition eliminated wall-shear and reduced vorticity generation and its effect on the downstream flow. A simplified fuel inlet boundary condition was applied and a constant heptane vapor mass flow rate of 0.00234 kg/s was imposed on the burner. A resulting time-averaged chemical heat release rate of 116.3 kW in the simulations matched the experimental estimate. The entrained air from the open boundary was at 298.15 K, the ground and burner side were isothermal (at 298.15 K) and the burner surface was kept at the boiling point of heptane \((372 \text{ K})\).

3. Results and discussion

Results from the simulations are presented with description of the modeled fire properties, followed by comparisons of temperature and soot predictions with experimental data, and finally with comparison of incident heat flux with experimental measurement. All comparisons are made against data from the study of Klassen and Gore \([8]\) for a 0.3 m diameter heptane pool fire.

3.1. Flame structure

Instantaneous contours of temperature are shown in Fig. 2. Radiating sooting regions are superimposed on top of the fire. These regions of high soot concentrations occur on the large vortical structures where the flamelet structures \([7]\) are assumed to occur. At the bottom of the fire, near the burner, few sooting regions are present and the majority of soot formation takes place at the downstream locations. The soot shown in Fig. 2 occurs on the flame-sheet, i.e. where instantaneous heat release rate is taking place. This is because the flamelet model provides the instantaneous emission from the flame-sheet \([15]\) which is converted to an equivalent soot volume fraction using the instantaneous resolved temperature, \(T\), and the modeled variance, \(T^2\).

Time-averaged values of overall radiant fraction (predicted value 0.30) and flame height (predicted value 1.39 m) compare well against experimental measurements of radiant fraction (= 0.31) and flame height (= 1.31 m), respectively.

![Fig. 2. Instantaneous contours of temperature showing vortical structures with overlaid regions of radiating soot.](image)

Centerline mean vertical velocity and temperature rise are compared with the McCaffrey correlation \([23]\) and experimental data \([8,24]\) in Fig. 3. The three flow regions—flame, intermittent and plume—are captured by the model. Vertical velocity in the intermittent and plume regions is well predicted consistent with the results of Wang et al. \([5]\), but is found to be lower than the correlation in the flame region. Closer to the pool surface, as discussed by McCaffrey \([23]\), velocity data are unreliable due to bias introduced by the large inlet area of the bi-directional probes used. In this region, where the flow is transitional \([8]\), LDV data from Weckman and Strong \([24]\) compare favorably with our model predictions.

Time-averaged temperature contours are shown in Fig. 4. In Fig. 4(a), resolved temperature, \(\langle T \rangle\), shows peak values of \(\sim 1300 \text{ K}\) occurring in the middle section of the fire with lower temperatures close to the burner. RMS temperature values, \(\sqrt{\langle T^2 \rangle}\), in Fig. 4(b) have a peak in
the upper regions of the fire where large scale fluctuations of heat release occur. Relative to the resolved temperature downstream of the fire, the peak RMS values are at most 50% of the resolved temperature or \( \sim 500 \text{ K} \). The modeled subgrid fluctuations of temperature, i.e. their variance, \( \sqrt{\langle T'^2 \rangle} \), have smaller peak values in the range of \( \sim 300 \text{ K} \) occurring closer to the burner, where the combustion process is not resolved by the LES grid and the resulting temperature gradients are large. The impact of the temperature variance on soot volume fraction prediction is discussed below.

Figure 5(a) shows the distribution of the volumetric emission, \( \langle \dot{q}_v \rangle \). Peak values of \( \sim 1 \text{ MW/m}^3 \) occur in the middle section of the fire with the lowest regions of the fire, close to the burner, not showing significant emission. Figure 5(b) shows the distribution of soot volume fraction, \( \langle f_s \rangle \), with high values occurring in the upper regions of the fire. Except for immediately downstream of the burner on the centerline, the RMS soot volume fraction, \( \sqrt{\langle f_s'^2 \rangle} \), also is not significantly high in the upstream locations, except on the outer periphery of the flame-sheet, see Fig. 5(c). The RMS values in the upper regions of the fire are an order of magnitude higher compared to the mean which is the result of high observed intermittency in the simulations. Peak values of \( \sim 3 \text{ ppm} \) are higher than the peak recorded experimental values (\( \sim 1.5 \text{ ppm} \)) for heptane [8].

3.2. Radial temperature distribution

Next, predicted temperature profiles are compared with experimental data [8]. In Fig. 6, time-averaged radial profiles of resolved temperature, \( \langle T \rangle \), and its RMS values are reported at several

![Image](https://example.com/image.png)

**Fig. 4.** Time-averaged contours of temperature: (a) resolved mean, (b) resolved RMS, and (c) subgrid modeled RMS (variance).

![Image](https://example.com/image.png)

**Fig. 5.** Time-averaged contours of (a) \( \langle \dot{q}_v \rangle \), (b) soot volume fraction, \( \langle f_s \rangle \), and (c) RMS soot volume fraction, \( \sqrt{\langle f_s'^2 \rangle} \).

![Image](https://example.com/image.png)

**Fig. 6.** Radial distributions of (a) predicted temperature, \( \langle T \rangle \), and (b) its RMS value \( \sqrt{\langle T'^2 \rangle + \langle r'^2 \rangle} \), the resolved RMS component \( \sqrt{\langle T'^2 \rangle} \) and the modeled subgrid RMS component \( \sqrt{\langle r'^2 \rangle} \), compared against experimentally estimated values [8] at various non-dimensional heights, \( h/D \), where \( D \) is the burner diameter.
heights. The RMS values comprise of the resolved component, $\sqrt{\langle T^2 \rangle}$, and the subgrid modeled variance, $\sqrt{\langle T'^2 \rangle}$. Comparisons are made at four heights, from $h/D = 0.2$ to $h/D = 4.2$, where $h$ is the height above the burner and $D = 0.3$ m is the burner diameter. At $h/D = 0.2$, which is the location where the flame necking phenomenon takes place, the predicted temperature is lower than the experimentally estimated values. At $h/D = 1.5$ and $3.4$, the temperature predictions are comparable to the experimental data whereas at the top of the fire, $h/D = 4.2$, temperatures are over-predicted. The RMS temperature at $h/D = 0.2$ are under-predicted for $r/D < 0.3$. Both the resolved RMS and modeled variance values are low in this region as can be observed in Fig. 6(b). This difference between the predicted and experimental RMS values indicates that the model is not able to capture the necking/flame-flapping behavior accurately. The RMS component at higher heights are generally in agreement with the experimental data, except at $h/D = 4.2$ where they are higher by over 100% on the centerline.

3.3. Absorption and soot distributions

Inclusion of absorption in the RTE solution is made possible with estimation of the absorption coefficient (see Eq. (2)). Predicted maximum value of absorption coefficient in the fire is $\sim 1.0 \text{ m}^{-1}$. Although inclusion of absorption does not significantly affect the overall radiant emission from the fire, local absorption effects can be observed in Fig. 7 in which radial distributions of the ratio between volumetric absorption and emission are shown. At the bottom of the fire, absorption can be up to 30% of emission, reducing the radiant loss near the burner. However, for the middle section of the fire, the ratio is $\sim 0.1 - 0.15$. The contribution of absorption is observed to decrease at the top of the fire.

In the experiment a three-line technique [8] was applied with wideband emission intensities recorded at 0.9 $\mu$m $\pm$ 50 nm and 1.0 $\mu$m $\pm$ 50 nm halfwidths and transmittance of a laser beam at 0.632 $\mu$m. The laser transmittance was used to estimate the soot volume fraction using the Rayleigh limit for small particles and the contribution of gas-phase radiation was neglected in the estimation process. The emission measurements provided volume fraction of hot soot. Since the flamelet based model [7] provides emission from hot soot, comparison of the estimated equivalent soot concentration can be easily made against the experimental data. The flamelet model also provides estimates of unoxidized soot released from the flame-sheet [15]. In future studies, the cold soot concentration can be compared against estimates from absorption based measurements for toluene [8].

Estimated soot volume fractions, $\langle \tilde{f}_v \rangle$, (see Section 2.2.2 for details) are compared against experimental measurements in Fig. 8(a). $\langle \tilde{f}_v \rangle$ are generally over-predicted at all heights, except at $h/D = 4.2$ where the predictions are lower than experimentally estimated values. Results from three cases with $C_{\text{TRI}} = 0.0$ (no TRI) and $C_{\text{TRI}} = 1.25$ and 2.5 (TRI included) are discussed.

![Fig. 7. Radial distribution of the ratio between volumetric absorption, $\langle \kappa \rangle G$, and emission, $\langle \tilde{q}_v \rangle$](image_url)

![Fig. 8. Radial distributions of estimated (a) soot volume fraction, $\langle \tilde{f}_v \rangle$, and (b) its RMS value, $\sqrt{\langle \tilde{f}_v^2 \rangle}$, compared against experimentally estimated values [8] at various non-dimensional heights, $h/D$.](image_url)
When \( C_{\text{TRI}} = 0.0 \), the assumption is that the equivalent soot concentrations predicted by the model occur at the cell resolved temperature, which can be an incorrect assumption frequently selected in LES studies [25]. Excluding TRI, the predictions are higher, except at \( h/D = 0.2 \) for \( r/D < 0.15 \)—in this region TRI does not impact the predictions. This is primarily due to the under-prediction of the temperature variance close to the burner (see Fig. 6(b)). For \( C_{\text{TRI}} = 1.25 \), \( \langle f_r \rangle \) predictions improve, especially at \( h/D = 1.5 \) and 3.4, whereas at \( h/D = 0.2 \), improvement is observed for \( r/D > 0.25 \). Increasing \( C_{\text{TRI}} \) to 2.5, effectively biasing the predictions towards higher flame temperatures, improves the \( \langle f_r \rangle \) predictions further.

Predicted RMS soot volume fractions, \( \sqrt{\langle f_r^2 \rangle} \), are compared with experimental estimations in Fig. 8(b). RMS predictions are higher than experimental data, except at \( h/D = 4.2 \), indicating higher intermittency, but improve with increasing \( C_{\text{TRI}} \) values, especially at \( h/D = 0.2 \) where the \( C_{\text{TRI}} = 2.5 \) case provides the best comparison. Excluding TRI, differences in RMS soot predictions of up to 200% can be observed. For example, on the centerline at \( h/D = 4.2 \), the \( \langle f_r \rangle \) predictions are 0.29 ppm for \( C_{\text{TRI}} = 0 \), reducing to 0.19 ppm for \( C_{\text{TRI}} = 1.25 \) and 0.17 ppm for \( C_{\text{TRI}} = 2.5 \) (experimental value of 0.19 ppm). Similarly, at \( h/D = 1.5 \), the difference between the experimental value (0.17 ppm) and predictions improve when \( C_{\text{TRI}} \) value is increased—1.46 ppm for \( C_{\text{TRI}} = 0 \), 0.72 ppm for \( C_{\text{TRI}} = 1.25 \) and 0.53 ppm for \( C_{\text{TRI}} = 2.5 \).

An additional set of curves are included in Fig. 8(b) for the \( C_{\text{TRI}} = 2.5 \) case, where the predicted temporal data is filtered using a Butterworth filter (8th order, 125 Hz cutoff frequency). This filter was also applied to the experimental data [8]. The average time-step in the computations captures the high frequency content missing in the experimental data. Filtering removes the high frequency content from the computed data. With the filter applied, the RMS predictions improve at \( h/D = 1.5 \) and 3.4 heights. Marginal improvement is also observed at \( h/D = 4.2 \), but no effect is seen for \( h/D = 0.2 \) indicating closer to the burner high frequency oscillations are not significant. A similar observation is made for the RMS component of temperature near the burner (see Fig. 6(b)). The low-pass filtering, expectedly, does not affect the mean soot volume fraction values.

### 3.4. Incident radiation

Finally, incident radiative heat flux at an axial location 0.825 m from the fire centerline is shown in Fig. 9. For the comparison with experimental data, 96 total solid angles were used. Data were also averaged for 20 s instead of the 120 s average for all results reported above, due to the longer computational times required using the 96 angles. The predicted incident heat flux showed a uniform axisymmetric distribution; however, ray effects were observed that are well known to occur with the application of the finite volume, discrete ordinates method (DOM) of RTE. The mean predicted heat flux compares well against the experimental data at heights up to 0.5 m above the burner, with slight over-prediction at higher heights up to ~2.0 m. Beyond 2.0 m the predictions agree with the experimental data. Between 0.5 m and 2.0 m, the over-prediction is due to the higher radiant emissions predicted from the flame sheet, as described above.

### 4. Conclusions

An optically-thin soot-radiation model [7] has been extended to include soot absorption for radiation calculations. With the application of this model, LES of a medium-scale heptane pool fire has been conducted. Predictions of the fire flowfield, temperature and soot volume fraction distributions as well as incident heat flux to an external location have been made.

Good agreement of predicted mean centerline vertical velocity and temperature rise with the McCaffrey correlation [23] and experimental data [8,24] was achieved. Predicted radial distributions of mean temperatures in the fire compared favorably against experimental measurements. The predicted RMS values compare well with experimental data as well, except near the burner. The estimated soot volume fractions qualitatively reproduce the data with positive and negative deviations in some locations. Their RMS values are significantly higher compared to experimental estimates. The contribution of TRI is demonstrated to be important in soot predictions, and predicted incident heat flux compares well against experimental measurement.

Improvements in turbulent combustion and subgrid temperature variance modeling would
have a positive impact on emission predictions and therefore soot estimations. In the future, modeling of toluene with comparison of cold soot predictions from the flamelet model against experimental data is planned. The prediction of cold soot near the burner is important in the case of sootier fuels like toluene and for larger scale pool fires where heat feedback to the pool is reduced due to the presence of a layer of cold soot on top of the burner [8]. Absorption modeling involving cold soot, therefore, will be a crucial aspect of modeling toluene fires.

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