ON THE MODELLING OF RADIATIVE HEAT TRANSFER IN LABORATORY-SCALE POOL FIRES

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Abstract

Two synthetic 30cm-diameter pool fires, generated from experimental data concerning mean and variance of temperature and soot volume fraction, are used to assess different radiative properties models. The first pool fire involves toluene while the second one is generated reducing the soot volume fraction by one order of magnitude in order to study the effects of optical thickness and radiation of gaseous species. Turbulence radiation interactions (TRI) are accounted for in a simplified manner, by considering the Optically Thin Fluctuation Approximation (OTFA) and by assuming that the emission soot volume fraction and the temperature are statistically independent. Decoupled radiative computations are carried out with the Finite Volume Method (FVM) by using the Statistical Narrow Band Correlated k method (SNBCK) and the Full Spectrum Correlated k model (FSCK). Full spectrum (FS) k-distributions are assembled from 43 and 367 narrow band (NB) databases. It is found that the FSCK can be used with confidence in such problems with a 5-point Gauss-Legendre quadrature scheme and k-distributions assembled from the 43 NB database, allowing a reduction in CPU time by a factor of 14 as compared to the 43 band SNBCK. Finally the effects of the OTFA and of correlations between the emission soot volume fraction and temperature are analyzed and quantified.

Introduction

Hydrocarbon pool fires with diameters larger than 0.3m burn with few exceptions in a predominantly radiative regime, where gaseous species (fuel and combustion products such as CO, CO₂, H₂O, CH₄) and soot are the radiatively participating species [1]. The difficulty in modeling the radiative heat transfer in pool fires arises from two distinct points.

The first difficulty is the spectral nature of gaseous species and soot. Simplified gray models are often considered in CFD simulations of fire problems, since implementing more sophisticated models may become extremely time consuming when fluid flow/combustion/radiative heat transfer are coupled [2]. However simple benchmarks have demonstrated that the gray assumption leads to poor predictions of the radiative heat transfer in combustion situations [3-5]. In an opposite way, more sophisticated NB models such as the Statistical Narrow Band (SNB) and the Correlated-k (CK) method were applied to fire problems [6, 7]. These methods have proven to be very accurate but they are probably too time consuming to be used in CFD simulations, despite the development of procedures which significantly improve their computational efficiency [3, 7]. Global models, such as the Weighted-Sum-of-Gray-Gases (WSGG) [8], the Spectral-Line-Based Weighted-Sum-of-Gray-Gases (SLW) [9] and the Full-Spectrum k-distribution (FSK) [10], provide potential compromises between these two approaches. They consist in replacing the non-gray gas by a number of gray gases, for which the radiative rates are computed independently. Although Dembele et al. [11] and Bressloff [12] found that the WSGG model provide a reasonable agreement as compared to NB models, other studies concluded that this method cannot be used with confidence over a wide range of soot loadings [3-5]. The SLW and the FSCK,
which can be viewed as improvements on the WSGG, have emerged in the last decade. They consist in reordering the absorption coefficients over the entire spectrum into a smooth, monotonically increasing function called the FS $k$-distribution. As shown by Modest [8], SLW and FSK models differ in the methodology employed to perform the integration of these $k$-distributions. The SLW uses a simple trapezoidal scheme, defining $N_G$ gray gases, whereas the FSK uses a quadrature scheme. Solovjov and Webb [13] and Modest and Riazzi [10] developed models to generate a single FS $k$-distribution for a mixture of gases and soot. A recent benchmark revealed that the mixing scheme of Modest and Riazzi must be used to achieve a good accuracy [5].

The second difficulty is relative to the turbulent fluctuations of scalars, such as the temperature, the mole fractions of gaseous species and the soot volume fraction which affect the radiative heat transfer through TRI. In CFD fire simulations TRI are generally ignored or treated in an oversimplified manner [3]. For a medium composed only of gaseous species, the absorption TRI can be in a first approximation ignored while the emission TRI can be handled accurately by coupling a presumed probability density function (pdf) approach with the concept of “laminar flamelet” [14]. The presence of soot adds difficulties since the OTFA may not be necessarily a good approximation and the modeling of emission TRI requires a joint pdf of temperature and soot volume fraction [14]. Experimental studies have provided measurements of instantaneous temperature and soot volume fraction, as well as the statistics related to these quantities. Sivathanu et al. [15, 16] measured instantaneous soot volume fraction by emission and absorption on heavily sooty jet and buoyant flames. They found differences between the soot volume fractions based on emission and those based on absorption, revealing the presence of large quantities of cold soot at all positions. The same observations were obtained by Grizo et al. [17] and by Murphy and Shaddix [18] in the case of large scale pool fires. Sivathanu et al. [15, 16] and Murphy and Shaddix [18] found in addition that emission soot volume fraction and temperature are negatively correlated in the under-fire region, with inter-correlation factors in the range -0.6 / -0.5 and greater than -0.3, respectively. Emission soot volume fraction proved particularly interesting since they allow successful prediction of the spectral radiation intensity [15]. On the contrary, predictions of the spectral radiative intensity based on extinction measurements were found to largely overestimate the experimental data [15].

The aim of the study is twofold: firstly to assess the validity of the FSCK method in the simulation of pool fires and to provide ways to improve its computational efficiency. This task is accomplished by using two synthetic pool fires, by neglecting absorption TRI and by assuming that emission TRI only results from the temperature self correlations. Secondly the influence of the OTFA and correlations between soot volume fraction and temperature are analyzed.

Models

- Synthetic Fire Plumes

Axisymmetric synthetic fire fields were created from experimental data obtained for a 30cm diameter toluene pool fire by Klassen and Gore [1] as previously made by Krishnamoorthy [19]. The experimental data of Klassen and Gore [1] were complemented by correlations to describe the spatial variations of mean excess temperature ($\Delta T$), standard deviation of temperature ($T_{rms}$) and mean soot concentrations ($f_s$) within the fire plume. First, the centerline variations (denoted by the subscript CL hereafter) of these variables were determined by fitting the centerline experimental data with cubic splines. Radial variations of the mean temperature were fitted using the formulations of Zhang et al. [20] which involve the normalized coordinates $z' = z / Q_{pool}^{2/5}$ (m.kW$^{-2/5}$) and $x = r / R_{pool}$, where $(z,r)$ are the cylindrical
coordinates while $R_{pool}$ and $\dot{Q}_{pool}$ represent the pool radius and the heat release rate respectively.

$$\frac{\Delta T}{\Delta T_{CL}} = \begin{cases} \exp\left(\frac{z}{\sigma_1}\right) & \text{for } z' \leq 0.04: \exp\left[\frac{(x - x_m)}{\sigma_2}\right] \exp\left[-\left((x - x_m)/\sigma_2\right)^2\right] \quad (\text{for } x \geq x_m) \\ \exp\left(\frac{z}{\sigma_3}\right) & \text{for } z' > 0.04: \exp\left[-(r/\sigma_3)^2\right] \quad (\forall x) \end{cases}$$

(1)

The expressions for $x_m$, $\sigma_1$, and $\sigma_2$ are given in Table 1. The radial evolution of soot volume fraction was fitted using the expression proposed by Krishnamoorthy [19]. As recommended by Gore and co-workers [1, 15], only the soot volume fractions measured from emission will be used for computations:

$$\frac{f_s}{f_{s,CL}} = \exp\left[-\frac{r}{\sigma_3}\right] \quad \text{with } \sigma_3 = 0.014\dot{Q}_{pool}^{2/5}$$

(2)

Concerning the radial variations of the standard deviation of temperature, the following correlations were applied with the expressions for $C$, $x_{m1}$, $\sigma_4$, and $\sigma_5$ given in Table 1:

$$\frac{T_{rms}}{T_{CL}} = \begin{cases} C \exp\left[\frac{x_m^2}{\sigma_4}\right] \exp\left[-\left((x - x_m)/\sigma_5\right)^2\right] & \text{for } x \geq x_{m1} \\ C \exp\left[\frac{x_m^2}{\sigma_4}\right] & \text{for } x < x_{m1} \end{cases}$$

(3)

Table 1. Parameters of Eqs.(1) and (3).

<table>
<thead>
<tr>
<th>$T_{mean}$ [19, 20]</th>
<th>$T_{rms}$</th>
<th>$x_i$ [19]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x_m = \exp\left[0.9\dot{Q}_{pool} - 205\right]z'$</td>
<td>$x_{m1} = -0.255\ln\left(z' + 10^{-7}\right) - 0.4$</td>
<td>$x_{CO_2} = 7\left(\frac{T - T_a}{T_{ad} - T_a}\right)$</td>
</tr>
<tr>
<td>$\sigma_1 = 0.4 + x_m$</td>
<td>$\sigma_5 = 3.1659z'$</td>
<td>$\sigma_4 = 2.7832z^{0.7903}$</td>
</tr>
<tr>
<td>$\sigma_2 = 0.5 - 0.4x_m$</td>
<td>$\sigma_4 = 0.38 + 2.0848z^{0.7} + 0.3184 \left(z' &gt; 0.04\right)$</td>
<td>$x_{H_2O} = 4\left(\frac{\sigma_4 - T_x}{T_{ad} - T_x}\right)$</td>
</tr>
</tbody>
</table>

Figure 1: Radial profiles at different heights of: (a) the mean temperature, (b) the variance of the temperature, and (c) the mean soot volume fraction.

Figure 1 shows the radial profiles of the mean and standard deviation of temperature and of the mean $f_i$ for different axial locations along the plume axis. It can be observed that the fitted profiles represent well the experimental data. The expressions used to predict molar concentrations of CO$_2$ and H$_2$O are given in Table 1 with $T_{ad}$ and $T_x$ denoting the adiabatic (2338K) and the ambient temperatures respectively. Toluene is highly sooting and consequently the radiative heat transfer is, in this case, largely dominated by soot radiation as
demonstrated by Krishnamoorthy [19]. A second synthetic pool fire, denoted Pool 2 hereafter, is more representative of less sooting liquid fuel such as heptane for example [1]. It was designed to assess the effects of optical thickness and of gas radiation by dividing the soot volume fraction by a factor of 10 while keeping both temperature and gaseous species fields unaltered. For both pools, decoupled radiative heat transfer computations are carried out in axisymmetric configurations. The size of the computational domain is 0.45m×1.29m and cells outside the combusting region are set to \( T_\infty \).

**- Turbulence/Radiation Interactions (TRI)**

The radiative transfer equation (RTE) can be written as:

\[
\frac{dI_\eta}{ds} + \kappa_\eta \phi I_\eta = \kappa_\eta \phi I_{b\eta} \quad (4)
\]

where \( I_\eta, I_{b\eta} \) and \( \kappa_\eta \) are the radiative intensity, the Planck function and the absorption coefficient at wavelength \( \eta \) and \( \phi \) is an array of state variables of the medium properties \( (T, p, x_i, f_s) \).

A time average form of the differential RTE can then be written as:

\[
\frac{d\overline{I_\eta}}{ds} + \frac{\kappa_\eta \overline{I_\eta}}{Absorption\ TRI} = \frac{\kappa_\eta \overline{I_{b\eta}}}{Emission\ TRI} \quad (5)
\]

The second term on the left side of Eq. (5) can be expressed as \( \kappa_\eta \overline{I_\eta} = \kappa_\eta \overline{I_\eta} + \kappa_\eta \overline{I_\eta} \cdot \kappa_\eta \overline{I_\eta} \) is usually neglected based on the consideration that the local intensity is weakly correlated with the local absorption coefficient. For a medium composed only of gaseous species this approximation, commonly referred as OTFA, is not generally valid over the entire spectrum but in most of the cases it does not affect significantly the total radiation intensity [14]. The presence of soot may invalidate this approximation. This point will be discussed in the results and discussions section. The term on the right side of Eq. (5) represents the correlation between the absorption coefficient and the blackbody intensity. For a purely gaseous medium, it can be easily expressed by using a presumed \( pdf \) combustion model coupled with the laminar flamelet concept [14]. However, the presence of soot adds a complication. Let us consider that soot is the only radiatively participating species and that its monochromatic absorption coefficient can be expressed as \( \kappa_{\eta,s} = C_{\eta,s} f_s \) \( (C_{\eta,s}=4.9 \) in the present study). This term can then be evaluated by considering a joint \( pdf \) of temperature and soot volume fraction:

\[
\overline{\kappa_{\eta,s} I_{b\eta}} = \int_{T_{min}}^{T_{max}} \int_{f_{min}}^{f_{max}} C_{\eta,s} f_s I_{b\eta}(T)pdf(T, f_s)dTdff_v \quad (6)
\]

The use of a simple clipped bivariate Gaussian \( pdf \) requires the knowledge of the cross-correlation between the turbulent fluctuations of soot volume fraction and temperature. This is not the case for the present measurements and it will be assumed, based on the conclusions of Gore and Faeth [22] for heavily sooting flames, that emission TRI is mainly the consequence of temperature self-correlation, soot volume fraction and temperature being assumed to be statistically independent. This approximation will be also discussed in the results section. Based on the above assumptions, the time average RTE is written as:
\[
\frac{d\overline{\Omega}}{ds} + \kappa_{q_T} \overline{I}_{bq} = \kappa_{q_T} \overline{I}_{bq} \quad \text{with} \quad \overline{I}_{bq} = \int_{I_b(T)} I_b(T) p df(T) dT
\] (7)

\(pdf(T)\) is a clipped Gaussian pdf with lower and upper limits equal to the ambient temperature and the adiabatic temperature, respectively. The divergence of the radiative flux is then expressed as:

\[
\nabla \cdot \mathbf{q} = \int_0^\infty 4\pi \kappa_{q_T} I_{bq}(T) l \eta - \int_0^\infty \int_0^{2\pi} \kappa_{q_T} I_{bq}(T) d\Omega \approx \int_0^\infty 4\pi \kappa_{q_T} I_{bq}(T) l \eta - \int_0^\infty \int_0^{2\pi} \kappa_{q_T} I_{bq}(T) d\Omega \quad \text{d} \eta
\]
(8)

In the present study the RTE is solved by the FVM using the special mapping developed by Chui et al. [23] for axisymmetric configurations. The spatial resolution is of 1 cm and an angular mesh with 24×32 control angles is used.

- Radiative Property Models

Statistical Narrow Band Correlated-k (SNBCK) Method

The SNBCK model is based on subdividing the entire spectrum into NBs and introduces the concept of \( k \)-distribution, which is basically a reordering of the erratic spectral absorption coefficient into a monotonically increasing function. A detailed explanation of the method can be found in [8]. This model introduces two new variables, namely the distribution function \( f(\phi_b, k) \) and its cumulative distribution function \( g(\phi_b, k) \), given by:

\[
f(\phi_b, k) = \frac{1}{\Delta \eta} \int_{\lambda \nu} \delta \left[ \left( k - \kappa_{q_T}(\phi_b, k) \right) \right] d\eta \quad \text{and} \quad g(\phi_b, k) = \int_{k}^{k_0} f(\phi_b, k') dk', \quad \text{where} \quad \kappa_{q_T}(\phi_b, k)
\]

is the medium spectral absorption coefficient evaluated at a reference state \( \phi_b \), and \( k \) is an absorption coefficient variable. Since the function \( g(k) \) increases monotonically, integration over the \( g \)-space can be performed by using a Gauss quadrature scheme. A 7-point Gauss-Legendre quadrature scheme is used for the calculations. The cumulative distribution is obtained by using a Malkmus model where the SNB parameters are taken from the 367 and 43 NB databases of Soufiani and Taine [24]. Gas mixture is treated by using the mixing scheme developed by Modest and Riazi [10]. Considering a binary mixture composed of \( \text{CO}_2 \) and \( \text{H}_2\text{O} \), the following expression for the gas mixture is obtained:

\[
g_{\text{mix}}(k_{\text{mix}}) = \int_{k_{\text{mix}}=0}^{k_{\text{mix}}} \int_{k_{\text{mix}}=0}^{k_{\text{mix}}} H[k_{\text{mix}} - (k_{\text{CO}_2} + k_{\text{H}_2\text{O}})] d g_{\text{CO}_2} d g_{\text{H}_2\text{O}} = \int_{k_{\text{mix}}=0}^{k_{\text{mix}}} g_{\text{CO}_2} \left( k_{\text{mix}} - k_{\text{H}_2\text{O}} \right) d g_{\text{H}_2\text{O}}
\]
(9)

Full Spectrum Correlated-k (FSCK) Method

This method extends the NB CK distribution method by reordering the absorption coefficient on the entire spectrum. This task is accomplished by defining a FS Planck-function weighted-

\( k \) distribution \( f(T, \phi, k) = \frac{1}{I_b(T)} \int_{I_b(T)} \delta \left[ k - \kappa_{q_T}(\phi) \right] d\eta \) and a FS Planck-function weighted cumulative \( k \)-distribution \( g(T, \phi, k) = \int_{k}^{k_0} f(T, \phi, k) dk \). Due to the smooth nature of the cumulative function, the integration of the reordered wavenumber can be easily achieved with a simple integration scheme. In the case of non-homogeneous and/or non-isothermal media,
as for SNBCK model, the assumption that the absorption coefficient is scaled or correlated is applied introducing errors in the methods [10]. The FSCK leads to a reordered RTE in smoothly-varying $g_r$-space [10]:

$$
\frac{dT_s}{ds} = k(T_0, \phi_0, g_0) \left[ a(T, T_0, g_0) I(T) - I_s \right] \quad \text{and} \quad \bar{I} = \int_{T_s}^{T_0} dg_0 = \sum_{j=1}^{N_d} \bar{I}_{s_j} w_j
$$

(10)

In this study a Gauss-Legendre quadrature scheme is used and a parametric study is performed on the number of quadrature points. The reference state is defined here by the molar fractions of the gas species and by the soot volume fraction averaged over the flame volume $V$. Three different ways for computing the reference temperature are considered: 1) a volume-averaged temperature, 2) an emission weighted temperature based on mean temperature and 3) a time-average emission-weighted temperature.

$$
1): T_0 = T_{av} = \frac{1}{V} \int_V T dV; \quad 2): T_0 = T_{em} = \frac{1}{V} \int_V k_p(\phi) T^5 dV; \quad 3): T_0 = T_{emT} = \frac{1}{V} \int_V k_p(\phi) T^5 dV
$$

(11)

The FS k-distributions are assembled from the 367 and 43 NB databases of Soufiani and Taine [24]. The Modest and Riazi [10] mixing scheme is used to obtain single FS k-distributions including participating gas species and non-gray soot. The procedure to generate the FS k-distributions can then be summarized as follows: firstly on each NB the single k-distributions for the gas mixture are generated by using Eq. 9. Secondly the absorption coefficient of soot is added to the NB cumulative k-distributions. Finally the single FS k-distributions are assembled from the previously computed single NB k-distributions by using the following relationship [10]:

$$
g(T, \phi, k) = \sum_{j=1}^{N_d} I_{b_j}(T) g_j(\phi_0, k) \quad \text{with} \quad I_{b_j}(T) = \int_{\Delta \eta_j} I_{b_j}(T)d\eta \approx I_{b_j}(T) \Delta \eta_j
$$

(12)

It is possible to neglect the weak dependence of spectral line broadening on species mole fractions, then the absorption coefficients are linearly dependent on species mole fractions. Using this approximation, single NB k-distributions were pre-calculated for 23 temperatures in the range 300-2500K, taking advantage that the mole fraction ratio of gaseous species is fixed in the present computations. This procedure may be used to avoid the computation of the expensive mixing process during a CFD simulation [24].

**Results and Discussions**

- Radiative Property Models

Figure 2 shows the divergence of radiative flux along the plume axis, the incident radiative heat flux on the pool surface and the incident radiative heat flux at a distance $r=0.45m$ from the pool center predicted by using the SNBC 367. Results obtained with the SNBC 43 are not shown since they are in very close agreement with those obtained with the SNBC 367 (see Table 2). Experimental data relative to the radiative feedback to the toluene pool surface are also represented.
Figure 2: Radiative outputs computed with the SNBCK 367 for a) the toluene pool fires and b) pool 2. LF, CF, and IF denote the laminar, the continuous and the intermittent flame regions. No TRI means that the absorption coefficient and the blackbody intensity in Eq. (5) are estimated by considering the mean value of scalars \( T, x_i, f_i \). The index 3 represents the results for an incident radiative heat flux at a distance \( r=0.45 \text{m} \) from the pool center.

Table 2. Error estimation (%) for the output of the radiative models when TRI is considered. Error estimators are defined as \( E_{r,\text{mean}} = \sum_i E_{r,i} / N \) and \( E_{r,\text{max}} = \max_{i=1,N} |E_{r,i}| \), where \( N \) is the number of mesh points and \( E_{r,i} = (\phi_i - \phi_{r,i}) / \phi_{r,i} \) and. The SNBCK367 is taken as reference. The third column represents the CPU time ratio between the current model and the SNBCK 367.

<table>
<thead>
<tr>
<th>Models</th>
<th>Pool</th>
<th>CPU ratio</th>
<th>Feedback</th>
<th>( \vec{v} \cdot \vec{q}_{\text{rad}} )</th>
<th>( \dot{q}_{\text{inc}} ) at ( r=0.45 \text{m} )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>\text{max}</td>
<td>\text{mean}</td>
</tr>
<tr>
<td>SNBCK43</td>
<td>Toluene</td>
<td>1/11</td>
<td>0.14</td>
<td>0.10</td>
<td>0.15</td>
</tr>
<tr>
<td></td>
<td>Pool 2</td>
<td></td>
<td>0.64</td>
<td>0.48</td>
<td>0.61</td>
</tr>
<tr>
<td>FSCK367</td>
<td>Toluene</td>
<td>1/26</td>
<td>2.98</td>
<td>1.02</td>
<td>2.82</td>
</tr>
<tr>
<td></td>
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<td>7.46</td>
<td>3.57</td>
<td>7.10</td>
</tr>
<tr>
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<td>1/134</td>
<td>2.28</td>
<td>0.66</td>
<td>2.71</td>
</tr>
<tr>
<td></td>
<td>Pool 2</td>
<td></td>
<td>6.91</td>
<td>2.98</td>
<td>6.64</td>
</tr>
</tbody>
</table>

Model results obtained by accounting the TRI are found to be consistent with the data, which underlines the relevance of using synthetic pool fires to assess the validity of radiative models in view of implementation in CFD simulators. Simulations were also carried out considering soot as gray particles with a Planck mean absorption coefficient based on local...
temperature. Results show that this approximation is appropriate for ‘Pool 2’ (Fig. 2b) but becomes questionable as the optical thickness increases. In the case of the toluene pool fire (Fig. 2a) it leads to an over-prediction of the radiative feedback to the fuel surface and for incident radiative flux at \( r=0.45\text{m} \) of about 15% whether the TRI are accounted for or not. Finally the effect of emission TRI based on temperature self-correlations leads to a large enhancement of the radiative losses for both flames, increasing significantly the radiative feedback to the pool surface and the incident radiative flux at \( r=0.45\text{m} \).

Figure 3 compares the incident heat flux in \( r=0.45\text{m} \) obtained by the FSCK with those obtained with the SNBCK 367 when emission TRI is considered. In Table 2 is summarized a detailed error estimation. The notations FSCK367 and FSCK43 indicate that the FS k-distributions were assembled using either the 367 NB database or the 43 NB database. As shown in Table 2, the FSCK is much more computationally efficient than the SNBCK, especially when the 43 NB database is used to assemble the FS k-distributions. Figure 3 and Table 2 show that solutions obtained with FSCK367 and FSCK43 agree well with the reference solutions when \( T_0=T_{\text{coll}} \) and \( N_G=10 \). These results show clearly that the FSCK, used in conjunction with the Modest and Riazzi [10] mixing scheme to assemble the FS k-distribution, is able to capture the non-gray nature of both soot particles and gaseous species. The influence of \( T_0 \) on the radiative output data is shown in Figure 3a, demonstrating that a time average weighted emission temperature must be used to achieve accurate predictions when TRI is considered. Figures 3b and Table 3 show the effects of \( N_G \) on the solutions. Predictions are found to remain satisfactory with only 5 quadrature points. Table 3 shows that the computational saving as compared to \( N_G=10 \) is only of 15% since a great part of the CPU time is devoted to assemble the FS k-distributions. Nevertheless, a decrease in \( N_G \) might result in a higher computational saving for 3D simulations, where the time required for solving the RTE increases drastically.

Table 3. Effects of the \( N_G \) on FSCK 43 predictions. Error estimators are defined as in Table 2. The third column represents the CPU time ratio between the current model and the FSCK 43 with \( N_G=10 \).

<table>
<thead>
<tr>
<th>( N_G )</th>
<th>Pool</th>
<th>CPU ratio</th>
<th>Feedback</th>
<th>( \vec{V} \cdot \vec{q}_{\text{rad}} )</th>
<th>( \dot{q}_{\text{inc}} ) at ( r=0.45\text{m} )</th>
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</thead>
<tbody>
<tr>
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<td>Toluene</td>
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<td>mean</td>
<td>max</td>
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<tr>
<td></td>
<td>Pool 2</td>
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<td>2.37</td>
<td>0.68</td>
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<td>2.46</td>
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<td></td>
<td></td>
<td>16.10</td>
<td>12.20</td>
<td>15.40</td>
</tr>
</tbody>
</table>

- Further discussions on TRI

This section is an attempt to analyze the effects of the OTFA and of the assumptions that soot volume fraction and temperature are statistically independent. The Reynolds averaging procedure is applied to the RTE (Eq. 4) integrated along a line of sight:

\[
\overline{I_{\eta}} = I_{\eta 0} \exp \left[ -\int_{0}^{\infty} \kappa_{\eta} ds' \right] \exp \left[ -\int_{0}^{\infty} \kappa_{\eta} I_{b\eta} ds' \right] \exp \left[ -\int_{0}^{\infty} \kappa_{\eta} ds'' \right] \exp \left[ -\int_{0}^{\infty} \kappa_{\eta} I_{c\eta} ds'' \right] ds' \\
+ \int_{0}^{\infty} \exp \left[ -\int_{0}^{\infty} \kappa_{\eta} ds'' \right] \left[ \kappa_{\eta} I_{b\eta} \right] \exp \left[ -\int_{0}^{\infty} \kappa_{\eta} ds'' \right] ds''
\]

(13)
Figure 3: Comparison between FSCK and SNCB: a) effects of the number of bands on the generation of the FS k-distribution and of the definition of the reference temperature, and b) effects of the number of quadrature points for 1) toluene pool fire and 2) Pool 2.

When OTFA is applied, terms $A_1$ and $A_2$ in Eq. (13) are equal to 1, while term $C$ is zero. The influence of OTFA is quantified by considering $A = \exp \left[ - \int_0^{R_{pool}} k_{\eta}^* (s^*) ds^* \right]$ which represents the attenuation of radiation emitted from the center of the pool fire. This is due to the absorption coefficient fluctuations by assuming that individual eddies are homogeneous and statistically independent and by dividing the line of sight in segments of length, $L$, larger than the integral length scale of turbulence (estimated to be 2 cm from the works of Klassen and Gore [1]) in order to avoid treating spatial correlations, this expression yields:

$$
\exp \left[ - \int_0^{R_{pool}} k_{\eta}^* (s^*) ds^* \right] \approx \prod_{i=1}^{N} \exp \left[ - \kappa_{\eta}^* \eta L \right] = \prod_{i=1}^{N} \int_0^{f_{s_{\max}}} \exp \left[ - C_{\eta,s} \eta (f_s - f_s^0) L \right] pdf(f_s) df_s (14)
$$

where $pdf(f_s)$ is a clipped Gaussian pdf computed from the mean and the variance of soot volume fraction reported by Klassen and Gore [1]. Figure 4 shows the spectral evolution of this quantity at different heights for the two pool fires considered. As mentioned by Coelho [14], the turbulent fluctuations of the absorption coefficient increase the transmissivity of the medium, implying $A \geq 1$. OTFA is expected to be valid when $A$ is close to 1. Results in Fig. 4b show that OTFA is a good approximation for pool 2 whatever the part of the flame considered and for the toluene pool fire in the intermittent flame region. However, in lower parts of the toluene pool fire ($z=0.11$m), the term $A$ is much larger than 1 for wavelengths lower than 2.1 $\mu$m, which suggests that the OTFA must be used with care in this part of the flame.

The cross correlation between fluctuations of the emission soot volume fractions and fluctuations of temperature is defined as $R = \int f_s T / \sqrt{f_s^2 \sqrt{T^2}}$. In CFD simulations the effects of correlations between temperature and soot volume fraction can be estimated by using a pdf composition method [25]. However, a simple physical analysis may be used to get insights. In the under-fire region, temperature is primarily a function of the mixture fraction and of the
enthalpy defect resulting from radiative losses, whereas the soot volume fraction is not expected to be well correlated with the mixture fraction within this part of the flow [26, 27].

As mentioned by Kollmann et al. [27] these cross correlations are thus the consequences of the radiative heat transfer. Based on this analysis, soot volume fraction and temperature are expected negatively correlated in the under-fire region where hot soot emits radiation. A fluctuation that locally increases (decreases) the soot volume fraction implies greater (lesser) radiative losses and then a decrease (increase) in temperature. This trend was quantified experimentally by Sivathanu and co-workers [15, 16] and by Murphy and Shaddix [18] and numerically by Kollmann et al. [27]. On the radiative heat transfer point of view, negative cross-correlations should reduce the effects of temperature fluctuations and then limit emission TRI [14]. Concerning the magnitude of the cross correlations, it can be argued that they should vary across the flame with strongest negative values in regions where the radiative losses are the most important. The computations provided by Kollmann et al. [27] in ethylene jet flames sustain this point. Based on the same analysis they should become globally more important as the ‘sooting’ nature of the fuel increases. The effects of cross correlations between soot volume fraction and temperature are here quantified by computing the emission term of Eq. 8 at different locations in the toluene pool fire for various values of $R$. A bivariate clipped Gaussian pdf is used for this purpose:

$$E_{mf} = \int_0^\infty C_{\eta, s} i_s \overline{I_{f b}}(T) d\eta = \int_0^\infty \left[ \int_{T_a}^{T_f} \int_{f_a}^{f_b} I(T) pdf(T, f) dTdff \right] d\eta$$

This term will be compared to $E_0 = \int_0^\infty C_{\eta, s} i_s \overline{I_{f b}}(T) d\eta$ for which the TRI are ignored. $R=0$ corresponds to the case where soot volume fraction and temperature are statistically independent, implying that emission TRI is only related to temperature self correlation. Figure 5 shows the evolution of the ratio between $E_{mf}$ and $E_0$. It is found that TRI always increases emission whatever the values of $R$ in the range between -0.5 and 0.0, this increase being more important in the intermittent flame where temperature fluctuations are larger. The two curves show that the assumption of emission TRI dominated by temperature self correlation is reasonable for $R$ greater than -0.2. As $R$ decreases cross-correlation effects influences significantly the radiative heat transfer.

**Concluding Remarks**

Two synthetic lab-scale pool fires, characterized by differences in optical thickness of one order of magnitude, are used to assess the accuracy and the computational efficiency of the FSCK method as compared to the SNBC. The FS k-distributions were assembled from
The assumption following a large saving in CPU time.

- The FSCK is a good candidate to be implemented in Fire Simulators. It is demonstrated that predictions in close agreement with those provided with the SNBCK can be achieved by considering a 5-point Gauss-Legendre quadrature scheme. FS k-distributions can be assembled with the 43NB database without losses in accuracy as compared to the 367 NB database, allowing a large saving in CPU time. Finally the reference temperature must be redefined in order to account properly for the effects of TRI.
- The absorption TRI is found to be negligible for the laboratory-scale flames with the exception of the lower part of heavily “sooting” flames at short wavelengths, implying that OTFA is a fairly good approximation. This conclusion is consistent with the one drawn by Mehta et al. in jet flames [25].
- Correlations between soot volume fractions and temperature limit TRI emission, especially when they are lower than -0.2. As a consequence, the assumption that the TRI emission is dominated by temperature self correlation should be used with caution. This point still requires further investigations.

![Image](image-url)

Figure 5: Effects $R$ on $E_m/E_0$ for means and variances of both temperature and soot volume fractions characteristic of intermittent (IF) and continuous flames (CF).

References