Modelling thermal radiation from one-meter diameter methane pool fires

J L Consalvi¹ and R Demarco¹²

¹ Université de Provence, IUSTI/ UMR CNRS 6595, 5 rue E. Fermi, 13453 Marseille Cedex 13, France
² Institut de Radioprotection et de Sûreté Nucléaire (IRSN), BP 3, 13115 St Paul-Lez-Durance, France

E-mail: jean-louis.consalvi@polytech.univ-mrs.fr

Abstract. The first objective of this article is to implement a comprehensive radiation model in order to predict the radiant fractions and radiative fluxes on remote surfaces in large-scale methane pool fires. The second aim is to quantify the importance of Turbulence-Radiation Interactions (TRIs) in such buoyant flames. The fire-induced flow is modelled by using a buoyancy-modified k-ε model and the Steady Laminar Flamelet (SLF) model coupled with a presumed probability density function (pdf) approach. Spectral radiation is modelled by using the Full-Spectrum Correlated-k (FSCK) method. TRIs are taken into account by considering the Optically-Thin Fluctuation Approximation (OTFA). The emission term and the mean absorption coefficient are closed by using a presumed pdf of the mixture fraction, scalar dissipation rate and enthalpy defect. Two 1m-diameter fires with Heat Release Rates (HRR) of 49 kW and 162 kW were simulated. Predicted radiant fractions and radiative heat fluxes are found in reasonable agreement with experimental data. The importance of TRIs is evidenced, computed radiant fractions and radiative heat fluxes being considerably higher than those obtained from calculations based on mean properties. Finally, model results show that the complete absorption coefficient-Planck function correlation should be considered in order to properly take into account the influence of TRIs on the emission term, whereas the absorption coefficient self-correlation in the absorption term reduces significantly the radiant fractions.

1. Introduction

The pool fire scenario represents a simplified version of fires that occur in practice. The numerical simulation of large-scale pool fires appears thus to be an important issue for fire safety purposes. Tiezen et al. [1] reported measurements of velocity in a methane pool fire with a diameter of 1 m. Xin et al. [2] and Cheung and Yeoh [3] provided large eddy simulations of these experiments by using simplified models to treat radiative heat transfer: Xin et al. [2] either used a constant radiant fraction method or a radiation model based on the finite volume method (FVM) coupled with a Gray-Wide Band (GWB) model whereas Cheung and Yeoh considered the discrete ordinates method with the grey assumption [3]. Nevertheless, the implementation of efficient methods to predict radiative heat transfer in large scale pool fires is a crucial issue since thermal radiation plays a major role in the heat transferred by such flames to the surroundings.

An accurate prediction of radiative heat transfer in turbulent flames is a difficult task since it requires a precise solution of the radiative transfer equation (RTE), a proper modelling of the spectral dependence of radiating species (radiatively participating gases and soot particles) and a proper
evaluation of the TRIs. The exact line by line method [4-6] as well as narrow band (NB) models, such as the statistical NB model [7] and the NB k-distribution method [8, 9], were implemented in CFD models to deal with combustion situations. However, they are probably too time-consuming for practical applications. The Full-Spectrum k-distribution (FSK) method [10], which extends the concept of the k-distribution over the entire spectrum, was found also to provide a reliable description of gas and soot radiation in combustion problems and is a good candidate to be implemented in CFD models [11].

Taking TRIs into account requires the modelling of two terms. The first term, known as ‘absorption TRI’, represents the nonlinear coupling between incident radiation and the local absorption coefficient. It is the consequence of property fluctuations across the domain. Its modelling is complex since it requires having a detailed knowledge of the instantaneous fields of temperature and species. Assuming that the local intensity is only slightly correlated with the local absorption coefficient this term can be ignored. This approximation, commonly referred to as OTFA, was found to be valid for a wide range of conditions [4-6, 12, 13], with the exception of very large-scale sooting jet flames where TRIs were found to reduce absorption by about 10% [14]. The second term, referred to as ‘emission TRI’, is determined on the basis of local properties only. It can be evaluated by using presumed pdf methods [15-19] or joint-probability transport models [4-6, 20-22].

The aim of this study is threefold: 1) to implement a comprehensive radiative model to predict both radiant fractions and radiative heat fluxes from methane pool fires produced by a burner with a diameter of 1 m for which the gas phase dominates radiation, 2) to quantify the importance of TRIs in the prediction of radiative heat fluxes in such flames, and 3) to determine the relative importance of different TRI-related terms. To the best authors knowledge, a comprehensive evaluation of the role of TRIs in large scale pool fires has not been reported in the past. The FSCK coupled with the mixing scheme of Modest and Riazzi [23] is used as the radiative property model. The OTFA is considered and a presumed-pdf approach coupled with the SLF model is applied to model TRI-related correlations.

The article begins with the presentation of the numerical model. Next, predicted radiant fractions and radiative heat fluxes on remote targets are compared with available experimental data. The effects of TRIs on predicted radiant fractions and heat fluxes are then discussed. Finally the conclusions drawn from the present study are summarized.

2. Numerical model

2.1. Flow field model
The numerical simulation of the turbulent flame flow fields includes the solution of the overall continuity equation, the Favre-Averaged Navier–Stokes equations in a low Mach number formulation, and transport equations for the turbulent kinetic energy, for the dissipation rate of turbulent energy, for the mixture fraction, $\xi$, for the mixture fraction variance, for the soot mass fraction, for the soot number density per unit mass of mixture, and for the total enthalpy. The conservation equations are solved in axisymmetric cylindrical coordinates using a finite volume method. For the convective terms, the ULTRASHARP approach is applied [24]. A second-order central difference scheme is used for diffusion terms. The pressure-velocity coupling is solved using the Iterative PISO algorithm [25]. Steady-state solutions are reached by time marching.

The production of turbulence due to buoyancy is modelled by a second-order expression [26, 27], whereas the effects of the anisotropy of turbulence due to buoyancy on the turbulent Reynolds stresses are introduced by using an algebraic stress model [28].

Turbulence-chemistry interactions are modelled by using the SLF model [29] coupled with a presumed-pdf of the mixture fraction, scalar dissipation rate ($\chi$), and enthalpy defect parameter ($X_R$) [30]. The flamelet library was generated by considering a detailed chemical mechanism consisting of 70 species and 463 reactions [31]. Statistical moments for scalar quantities can then be computed from the flamelet library and a joint pdf of the mixture fraction, scalar dissipation rate and enthalpy defect.
parameter. The statistical independence of $\xi$, $\chi$, and $X_R$ is assumed and the joint pdf is thus modelled as the product of a Beta function for the mixture fraction and two Dirac functions for both the scalar dissipation rate $[32]$ and the enthalpy defect parameter $[33]$.

The acetylene-based two-equation soot model proposed by Leung et al. is used $[34]$. The surface growth term is assumed to depend linearly on soot particle surface area. The kinetic constants in the nucleation and growth rates are $k_n = 10^4$exp$(-21000/T)$ s$^{-1}$ and $k_{SG} = 0.75 \times 10^3$exp$(-12100/T)$ m$^{-2}$s$^{-1}$. The oxidation of soot is attributed to OH and $O_2$. Soot oxidation by $O_2$ is given by the NSC model $[35]$ while soot oxidation by OH is based on the Fenimore and Jones model $[36]$. The rate of soot oxidation by OH is given by $k_{OH} = 1.27 \times 10^{-3}/\sqrt{T}$ m$^{-2}$s$^{-1}$ and the collision factor is assumed to be 0.08. Finally, the number of carbon atoms in the incipient soot particle is taken as being equal to 60 $[37]$ and the agglomeration rate is taken as being equal to 3 $[37]$.

2.2. Radiation Model

2.2.1. Radiative property model. In the present simulations only $CO_2$ and $H_2O$ are considered as gaseous radiatively participating species. The spectral soot absorption coefficient was determined using the small particle limit of Rayleigh scattering for a cloud of non-uniform particle size, leading to $\kappa_{g,S} = C_F S \eta$. $C$ is taken equal to 4.9 which is consistent with the value of the soot complex index of refraction, $m = 1.57 - 0.56i$, commonly used for reporting soot volume fraction measurements in flames. $F_S$ is the soot volume fraction and $\eta$ is the wavenumber.

The FSK method is used as radiative property model $[10]$. In this method the absorption coefficient is reordered over the entire spectrum by defining a Full-Spectrum (FS) Planck-function-weighted $k$-distribution, $f(T, \phi, k) = \frac{1}{I_b(T)} \int_0^\infty I_b(T) \delta[k - \kappa(\phi)] d\eta$, and a FS Planck-function-weighted cumulative $k$-distribution, $g(T, \phi, k) = \int_0^k f(T, \phi, k) dk$. In the latter definitions, $\kappa, k$ and $I_b$ represent the absorption coefficient, the absorption coefficient variable and the Planck function. Spectral quantities are indexed by $\eta$. $\delta$ is the Dirac function. $\phi$ is an array of state variables of the medium properties $(T, p, x_i, f_S)$ where $T$, $p$ and $x_i$ are the temperature, the pressure, and the molar fraction of the species $i$, respectively. Due to the smooth nature of the cumulative function, the integration of the reordered wavenumber can be easily performed with a simple quadrature scheme. In the case of non-homogeneous and/or non-isothermal media the assumption that the absorption coefficient is scaled or correlated is applied. In addition, a reference state of the medium properties must be defined to carry out the derivation. Quantities relative to the reference state are indexed by 0 in the following. In this study the FSCK formulation is considered, leading to a reordered RTE in the smoothly-varying $g_0$-space:

$$\frac{dI_g}{ds} = k^* (T_0, \phi_0, g_0) [a(T, T_0, g_0) I_b(T) - I_g]$$

where $a(T, T_0, g_0) = \frac{dI_g(T, \phi_0, k)}{dg_0(T, \phi_0, k)}$. $I_g$ represents the radiative intensity at a given cumulative $k$-distribution value. The total intensity, $I$, is then estimated as:

$$I = \int_0^1 I_g d g_0 \approx \sum_{j=1}^{N_G} I_{g_j} w_j$$

$N_G$, $g_j$ and $w_j$ are the number of quadrature points, the quadrature points and the corresponding weights respectively. Decoupled radiative heat transfer computations showed that $N_G$ can be set equal
to 5 without altering the quality of the results [38]. 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. In agreement with a previous work the reference temperature is computed as a time-averaged emission-weighted temperature [38].

The FS $k$-distributions are assembled from the 43 NB database of Soufiani and Taine [39] by using the Modest and Riazi mixing scheme [23]. It should be noticed that the use of the 43 NB database instead of the 367 NB database allows large computational savings without altering the quality of the solutions [38]. The procedure can be described as follows: firstly on each NB the single $k$-distributions for the gas mixture are generated by using the following expression:

$$g_{\text{mix}}(k_{\text{mix}}) = \frac{1}{T} g_{CO_2}(k_{\text{mix}} - k_{H_2O}) d\tilde{\sigma}_{H_2O}$$  \hspace{1cm} (3)

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:

$$g(T,\phi,k) = \sum_{j=\text{all NBs}} I_{bj}(T) g_j(\phi_j, k)$$  \hspace{1cm} (4)

Mixing at the NB level is demanding computationally. In order to further reduce the CPU time, mixture NB (MNB) $k$-distributions are pre-database for different values of $R = x_{CO_2}/x_{H_2O}$, and interpolations are carried out for mixtures of arbitrary species mole fraction ratios [40].

2.2.2. Turbulence Radiation Interactions. Equation (1) is time-averaged to account for TRIs:

$$\frac{d\overline{T_R}}{ds} + k^*\overline{T_R} + k^*\overline{I_g} = k^*\overline{T_0} + k^*\overline{I_0}$$  \hspace{1cm} (5)

The absorption term can be expressed as $k^*\overline{I_g} = k^*\overline{I_g} + k^*\overline{I_g}$. In the present study the term $k^*\overline{I_g}$ is neglected based on the OTFA. As discussed in the introduction, previous studies demonstrated that this approximation is adequate for weakly-sooting flames as considered in the present study. Mean values of the absorption coefficient and of the emission term are computed as:

$$k^* = \rho \int_{0}^{1} \frac{1}{\rho} \int_{0}^{1} \int_{0}^{1} k^* (\xi, \chi, X_R, f_s) \tilde{P}(\xi, \chi, X_R, f_s) d\xi d\chi dX_R df_s$$  \hspace{1cm} (6)

$$k^* aI_b = \rho \int_{0}^{1} \frac{1}{\rho} \int_{0}^{1} \int_{0}^{1} k^* (\xi, \chi, X_R, f_s) \alpha^* (\xi, \chi, X_R) I_b^* (\xi, \chi, X_R) \tilde{P}(\xi, \chi, X_R, f_s) d\xi d\chi dX_R df_s$$  \hspace{1cm} (7)

where the pdf is expressed as $\tilde{P}(\xi, \chi, X_R, f_s) = \tilde{P}(\xi) \delta(\chi - \tilde{\chi}) \delta(X_R - X_{R,\text{mean}}) \delta(f_s - \tilde{f}_s)$. $\tilde{\chi} = C_{v2} \frac{\bar{\epsilon}_R^{7/2}}{\kappa}$ and $X_{R,\text{mean}}$ are the local mean values of the scalar dissipation rate and of the heat loss fraction respectively. $C_{v2}$ is taken as being equal to 2 and $X_{R,\text{mean}}$ is computed as proposed by Brookes and Moss [33]. The present formulation neglects the influence of the fluctuations of soot volume fraction. This approximation may alter the evaluation of emission TRI since the soot absorption coefficient (soot volume fraction)-Planck function (temperature) correlation is ignored.
Nevertheless, it seems reasonable for the pool fires considered in the present study where the radiative heat transfer is dominated by the gas-phase contribution. This model will be referred to hereafter as Mod 1.

2.2.3. RTE Solver. The radiative transfer equation is solved by the Finite Volume Method (FVM) using the special mapping developed by Chui et al. for axisymmetric configurations [41]. Computations were carried out using the first-order STEP scheme for spatial discretization and a uniform angular mesh with 36x48 control angles.

3. Results and Discussions

3.1. Experimental and computational details

The two 1m-diameter methane pool fires with HRRs ($\dot{Q}$) of 49 kW and 162 kW, experimentally investigated by Hostikka et al. [42], were simulated. The corresponding dimensionless fire powers, given by $\dot{Q}_D^* = \dot{Q}/\rho_o C_p T_o \sqrt{gD^2}$, are of 0.044 and 0.14 respectively. In the previous expression $D$ and $g$ represent the pool diameter and the gravitational acceleration. The subscript $\infty$ refers to ambient conditions. In both cases the radiant fraction, $\chi_r$, was reported. The radial and vertical radiative heat flux profiles outside the flame region were measured. The vertical distributions were measured at 1m and 0.8m from the center of the burner for the 49 kW and the 162 kW pool fires, respectively. The radial distributions were measured along a radius on the plane aligned with the burner surface. Unfortunately no measurement concerning the flame structure was reported in the study of Hostikka et al. [42].

Figure 1 shows the fields of mean temperature. In the case of the 49 kW pool fire (figure 1a), the combustion is found to occur close to the burner. This follows the experimental observations of Zukoski [43] who pointed out that, when $\dot{Q}_D^* < 0.1$, the combustion region is divided into many flamelets that lean toward the axis of the source and that have flame lengths much smaller than the diameter of the source. Predicted flame heights are determined here as the location where the mean mixture fraction reaches its stoichiometric value (0.055 for methane in air). The flame height normalized by the burner diameter is of about 0.05, which is consistent with the data compiled by Zukoski [43] for small range of $\dot{Q}_D^*$.

As the normalized HRR is increased to 0.14 (figure 1b), the mean temperature field suggests that the classical description of a pool fire with a single continuous flame region, an intermittent flame region, and the inert plume is recovered. This behaviour is also in qualitative agreement with experimental observations which mention that the short flamelets are expected to merge and form a single flame for $\dot{Q}_D^* \approx 0.1$ [43]. The normalized flame length is 0.61, which compares rather well with the value of 0.8 computed from both the correlations of Heskestad [44] and Quintiere and Grove [45]. The correlations were applied by setting the radiant fraction, $\chi_R$, to 0.16 as measured by Hostikka et al. [42]. The numerical predictions of flame heights agrees also well with the data compiled by Zukoski [43], which show that measured normalized flame heights range from about 0.6 to 1 for $\dot{Q}_D^* \approx 0.14$.

3.2. Comparison with experimental available data

Hostikka et al. [42] reported radiant fractions of 0.08 and 0.16 for the 49 kW and the 162 kW pool fires with an uncertainty of 11%. Measured radiant fractions range thus from 0.071 to 0.089 and from 0.142 to 0.178 for the 49 kW and the 162 kW pool fires respectively. The corresponding predicted radiant fractions are 0.095 and 0.206, which compares favourably well with
the upper bounds of the experimental data. In addition these results show that the model reproduces
the increase in radiant fraction with $\dot{Q}_D$ correctly.

**Figure 1.** Mean temperature for: (a) the 49 kW pool fire and (b) the 162 kW pool fire.

Figure 2 shows the vertical and radial distributions of radiative flux. Predictions are in reasonable
agreement with the experimental data. Figures 2a$_1$ and 2b$_1$ show that in the vertical direction the
radiative heat fluxes reach a peak and then decrease rapidly. Calculated vertical profiles are found to
match closely the experiments. Figures 2a$_2$ and 2b$_2$ show that in the radial direction the radiative heat
flux decreases quickly as the radial distance increases. For the 162 kW pool fire the simulation
overpredicts the experiment near the burner whereas a more satisfactory agreement is obtained for
$r > 0.75m$ (see figures 2b$_2$). The largest discrepancies are observed for the 49 kW pool fire (see
figure 2a$_2$), where the heat fluxes are very low (not significant for fire safety purposes) and therefore
very sensitive to small errors in the flow field predictions.

3.3. Influence of TRI-related-terms on radiative outputs
This section discusses how the predicted radiant fractions and radiative heat fluxes on surrounding
surfaces are affected by considering different TRI closures for the absorption and emission terms. The
role of TRIs on radiative outputs can be better understood by isolating their effects on the radiation
calculations alone. As a consequence, decoupled radiation calculations are carried out by using the
flow field computed with the most complete model (Mod 1).

The different scenarios as well as the corresponding predicted radiant fractions are summarized in
table 1. The comparison between the calculations carried out with (Mod 1) and without TRIs (Mod 2)
shows clearly the strong influence of TRIs on the flame radiative losses. The radiant fractions are underpredicted by about 130% and 178% for the 49 kW and the 162 kW pool fires when TRIs are ignored. In addition, these results suggest that the enhancement in radiative losses due to TRIs increases with $\dot{Q}^*$. The comparison of the radiant fractions computed with Mod 2, Mod 3, Mod 4, and Mod 5 shows the effects of the different levels of closure on the emission term. In all these simulations the absorption coefficient in the absorption term is modelled from mean property values. In Mod 3 only the influence of TRIs on mean Planck function is considered. In Mod 4 the fluctuations of the absorption coefficient and of the Planck function are taken into account separately, but the correlation between the two is disregarded. Finally the most complete formulation, Mod 5, considers the effects of the correlation between the gas absorption coefficient and the Planck function. Results in table 1 reveal that accounting for the temperature self-correlation increases significantly the radiant fractions (Mod 2 vs. Mod 3) but its contribution alone is not sufficient to model correctly the emission term (Mod 3 vs. Mod 5). Mod 4 improves the predictions as compared to Mod 3 (Mod 4 vs. Mod 5). However the comparison between Mod 4 and Mod 5 shows that the gas absorption coefficient-Planck function correlation cannot be neglected. As discussed by Coelho [12] this correlation is positive, resulting in a large increase in the radiant fractions (Mod 5 vs. Mod 4) in the present cases. Finally, Mod 1 extends Mod 5 by considering the effects of the absorption coefficient self-correlation on the absorption term. This term contributes to enhance flame absorption leading to a non-negligible reduction in the radiant fraction (see table 1).

![Graphs showing heat flux predictions vs. experiments for different kW fires](image-url)

**Figure 2.** Predicted heat fluxes vs. experiments for (a) the 49 kW pool fire and (b) the 162 kW pool fire. The indexes 1 and 2 refer to the vertical distribution of heat flux and to the radial distribution of heat flux at $z=0$, respectively.
Figure 3 shows the effects of these different closures on the vertical and radial distributions of the radiative flux. A comparison between the simulations made with Mod 1 and Mod 2 shows that heat fluxes are severely underpredicted when TRIs are neglected: the peaks in the vertical direction are lower by factors of about 2.8 and 2.5 for the 49 kW and the 162 kW pool fires, whereas the radial distributions are also strongly underestimated. The predictions obtained with the other TRI scenarios follow the same trends as those observed for the radiant fractions (see table 1). Figure 3 shows also that the different closures modify the shape of the distributions. It can be observed that both predicted vertical and radial profiles are much flatter in absence of TRIs than when Mod 1 is considered.

Table 1. Effects of the different TRI closures on the radiant fraction. The values in brackets indicate the relative error (in %) defined as $E_r = \left( \chi_{R,\text{Mod1}} - \chi_{R,\text{model}} \right) / \chi_{R,\text{model}} \times 100$. Quantities denoted without an overbar refer to evaluations from mean variables, i.e. without accounting for TRIs.

| Test Case | Absorption | Emission | 49 kW | 162 kW |
|-----------|------------|----------|-------|--------|
| Exp.      | -          | -        | 0.08 (0.071-0.089)$^a$ | 0.16 (0.142-0.178)$^a$ |
| Mod 1     | $\overline{k}$ | $k \times a_{I_b}$ | 0.095 | 0.206 |
| Mod 2     | $k$        | $k \times a_{I_b}$ | 0.041 (131.7%) | 0.074 (178.4%) |
| Mod 3     | $k$        | $k \times a_{I_b}$ | 0.048 (97.9%)  | 0.103 (100.0%) |
| Mod 4     | $k$        | $\overline{k} \times a_{I_b}$ | 0.061 (57.3%) | 0.134 (53.7%) |
| Mod 5     | $k$        | $k \times a_{I_b}$ | 0.120 (-21%) | 0.223 (-7.6%) |

$^a$ the uncertainty on $\chi_R$ are estimated as 11%.

4. Concluding remarks

Two methane pool fires generated by a burner with a diameter of 1 m were simulated by using a buoyancy-modified k-ε model and the SLF model to model chemistry. The FSCK was applied to account for the non-grey nature of gas and soot radiation. TRIs were modelled on the basis of the OTFA; the emission term and the mean absorption coefficient were then closed by using a presumed pdf of the mixture fraction. In addition the importance of TRIs and the influence of different levels of closure for TRIs on the prediction of radiative losses and radiative fluxes on remote surfaces were quantified. The following conclusions can be drawn:

1. Predicted radiant fractions and radiative heat fluxes on remote surfaces are reasonable agreement with available experimental data when TRIs are considered.
2. TRI considerably enhance the radiative losses and the radiative heat fluxes on remote surfaces. Disregarding TRIs also significantly modifies the shape of both vertical and radial distributions of radiant flux.
3. The complete gas absorption coefficient-Planck function correlation should be considered in order to properly take into account the influence of TRIs on the emission term.
4. The effects of absorption coefficient self-correlation on the absorption term cannot be neglected. They contribute to increase the absorption and in turn to decrease the radiative losses and the heat fluxes on remote targets.
Figure 3. Effects of different TRI closures on radiative heat fluxes for (a) the 49 kW pool fire and (b) the 162 kW pool fire. The indexes 1 and 2 refer to the vertical distribution of heat flux and to the radial distribution of heat flux, respectively.

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