Evaluation of the Correlated-K and other Gas Radiation Models for Combustion Applications

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ABSTRACT

The correlated-k (CK) distribution gas model is evaluated for some typical fires and combustion applications. The method based on the cumulative distribution function of the absorption coefficient has been widely used for atmospheric applications, but little tested for combustion systems. The CK approach, suitable for mixtures of gases and scattering particles is applied in the current work to PMMA and natural gas fires. For comparison purposes, results obtained with the narrow band statistical (NBS) and weighted sum of gray gases (WSGG) models are also presented for the same scenarios. The results clearly show that the CK approach provides a good level of accuracy with acceptable CPU times for the fire configurations tested, in the prediction of radiative quantities.

KEY WORDS: radiation, gas models, correlated-k model

NOMENCLATURE

g	cumulative distribution function in gas model
I	intensity of radiation
k, κ_ν	gas absorption coefficient
$\overline{k_\nu}$	mean line-intensity to spacing ratio
L	thickness of the medium
N_q	number of quadrature points in CK gas model
P	gases total pressure
s	distance along a beam in the s direction
T	temperature or transmissivity
x	position variable
$\overline{\gamma_\nu}$	mean half-width of the absorbing lines inside $\Delta\nu$
$\overline{\delta_\nu}$	equivalent line spacing
$\Delta\nu$	wavenumber range
ν	wavenumber
σ	soot particles scattering coefficient
Φ	soot particle scattering phase function
χ	molar fraction
ω	weight of quadrature point g in CK method
Ω	solide angle

Subscripts

b	blackbody
g	relative to absorbing/emitting gases
j	relative to the j th quadrature point in the CK method
s	relative to soot particles
ν	spectral value

Superscripts

$\bar{}$	spectrally averaged

INTRODUCTION

In many fires and combustion systems, gas radiation represents an important mode of heat transfer. High temperatures are encountered in these systems and radiation is the main mode of heat transfer. Consequently, its modelling is of major importance for predicting temperatures, heat fluxes and other radiative quantities. Radiation calculations in combustion systems are complex due to the spectral structure of the combustion products, which are mainly mixtures of gases and soot particles. For predicting gaseous radiative properties, the line-by-line (LBL) method, although it is an exact approach, is rarely used in practical engineering because of its enormous computational cost. Some approximate models have been developed, based on the magnitude of the frequency interval, to quantify the gas radiative properties. The simple gray gas concept can lead to important errors in fire systems. The WSGG model, first introduced by Hottel and Sarofim [1] has been widely used by fire modellers because of its simplicity of implementation and low computational times. A more elaborate version of the WSGG model based on the absorption-line blackbody distribution function has been developed and tested against LBL model by Denison and Webb [2]. One of the main disadvantages of the WSGG model is the inability of the model to take into account the spectral dependence of wall radiative properties, which could lead to important errors. Spectral NBS models, describe the radiative properties of isothermal and homogeneous gases in terms of mean transmissivities averaged over spectral interval of typically 5 to 50 cm^{-1} [3, 4]. For non-homogeneous and non-isothermal mixtures, the Curtis-Godson (CG) or Lindquist-Simmons (LS) approximations are necessary. NBS models could lead to results that agree with line-by-line calculations with reasonable accuracy. However the NBS approach presents some disadvantages: (i) the CG and LS approximations may lead to inaccurate results [5], (ii) its description of the radiative properties of mixtures of gases and non-scattering particles in terms of transmissivity makes the NBS model difficult to use for radiative transfer when the scattering attenuation and gain terms are both to be

included. Despite some of the above mentioned disadvantages, WSGG and NBS models have never been discredited since they can provide satisfactory results depending on the physical situation being dealt with. Nevertheless there is a need for more accurate techniques that overcome their drawbacks and are suitable for a wider application. An alternative solution for mixtures of gases and particles media is the correlated-k (CK) distribution method widely used for atmospheric applications [3, 6]. The spectral CK method describes the gas properties in terms of absorption coefficients, which can be used with any solution method for the radiative transfer equation (RTE). The method can

be applied to non-homogeneous and non-isothermal mixtures of gases and absorbing-scattering particles. It could also be applied to homogeneous and isothermal mixtures without scattering. The CK method was applied to heat flux calculations, with the discrete ordinate method to a 1D combustion system [7]. However the CK method has been applied infrequently to combustion and fire applications. Few works have investigated the method for various practical engineering configurations and compare it to other models. The objective of the present paper is to help assessing the application of spectral CK method for typical combustion products, by comparing its solutions to other approximate methods such as the NBS and WSGG models, as well as to published experimental data. The analysis is carried out in terms of accuracy and CPU times, and the results discussed for some practical fires and combustion configurations. Both PMMA and methane fires are considered.

MATHEMATICAL MODELS

Correlated-k (CK) method

The concept of the CK method is to transform a frequency integration into an integration over the reciprocal function k(g) of the cumulative distribution function g(k). The transmissivity of an homogeneous and isothermal gas slab of length L, spectrally averaged over a spectral interval $\Delta\nu$, is

$$\overline{T_\nu} = \frac{1}{\Delta\nu}\int_{\Delta\nu} \exp(-\kappa_\nu L)d\nu = \int_0^1 \exp[-k(g)L]\,dg \qquad (1)$$

The advantage of using Eq. 1 is that unlike the gas spectral absorption coefficient κ_ν, the function k(g) has no fine structure and only a few N_q Gaussian quadrature points g_j of weight ω_j (7 in this study) are necessary to perform the integration. More generally in the CK formulation the spectrally averaged value of any function $F(\kappa_\nu)$ of the absorption coefficient is:

$$\overline{F_\nu} = \frac{1}{\Delta\nu}\int_{\Delta\nu} F[\kappa_\nu]d\nu = \int_0^1 F[k(g)]\,dg \cong \sum_{j=1}^{N_q} \omega_j F[k(g_j)] \qquad (2)$$

The transmissivity of a non-homogeneous and non-isothermal absorbing gas column, divided into M discrete homogeneous and isothermal paths of length L_i, and molar fraction χ_i is given in the CK formulation by:

$$\overline{T_\nu} = \sum_{j=1}^{N_q} \omega_j \exp\left(-\sum_{i=1}^{M} k_i(g_j)\chi_i P L_i\right) \qquad (3)$$

The main difficulty in the CK approach is the choice of the quadrature points in Eq. 2, and the determination of $k(g_j)$ since no explicit analytical expressions exist. In the present study, calculations of $k(g_j)$ values are based on a Newton-Raphson procedure [6, 7] using the gas parameters $\overline{K_\nu}$ (mean line-intensity to spacing ratio) and $\overline{\delta_\nu}$ (equivalent line

spacing) from [8]. Seven Gaussian quadrature points were found to be sufficient for CK calculations, after a preliminary investigation.
For a mixture of gases and absorbing, emitting and scattering soot particles, by spectrally averaging the RTE, the CK model gives:

$$\frac{dI_j(s,\Omega)}{ds} = -[k_{jg} + k_{vs} + \sigma_{vs}]I_j(s,\Omega) + [k_{jg} + k_{vs}]\overline{I_{bv}} + \frac{\sigma_{vs}}{4\pi}\int_{\Omega'=4\pi} I_j(s,\Omega')\Phi(\Omega,\Omega')d\Omega' \qquad (4)$$

where $k_{jg} = \chi_{H_2O} Pk_{H_2O}(g_j) + \chi_{CO_2} Pk_{CO_2}(g_j) + \chi_{CO} Pk_{CO}(g_j)$.

Equation 4 could be solved by using any solution method. In the current work the control volume technique is used and the following relation (integral approach) provides the intensity:

$$I_j(s,\Omega) = I_j(0,\Omega)\exp(-\beta_j s) + \int_0^s S_j(s',\Omega)\exp[-\beta_j(s-s')]ds' \qquad (5)$$

where $S_j = [k_{jg} + k_{vs}]\overline{I_{bv}} + \frac{\sigma_{vs}}{4\pi}\int_{\Omega'=4\pi} I_j(s,\Omega')\Phi(\Omega,\Omega')d\Omega'$ and $\beta_j = k_{jg} + k_{vs} + \sigma_{vs}$

Once the intensities I_j are found from the solution of Eq. 5, the spectrally averaged intensity $\overline{I_\nu}$ is expressed by:

$$\overline{I_\nu} = \frac{1}{\Delta\nu}\int_{\Delta\nu} I_\nu d\nu = \sum_{j=1}^{N_q} \omega_j I_j \qquad (6)$$

The in-scattering contribution [last term on the right hand side of Eq. 4], which is the most complex to model by the NBS or other gas models, is easily incorporated in the CK formulation.

Narrow-band statistical (NBS) model

In the current work, the NBS model is based on the Malkmus exponential-tailed-inverse line strength distribution model [4]. The spectrally averaged transmissivity of a homogeneous and isothermal gas layer of length L is:

$$\overline{T_\nu} = \frac{1}{\Delta\nu}\int_{\Delta\nu}\exp(-\kappa_\nu L)d\nu = \exp\left[-\frac{\overline{\beta_\nu}}{\pi}\left(\sqrt{1+\frac{2\pi\chi PL\overline{k_\nu}}{\overline{\beta_\nu}}}-1\right)\right] \qquad (7)$$

where $\overline{\beta_\nu} = 2\pi\overline{\gamma_\nu}/\overline{\delta_\nu}$ and $\overline{\gamma_\nu}$ is the mean half width given by:

$$\bar{\gamma}_{\nu H_2O} = \frac{P}{P_s}\left\{0.462\chi_{H_2O}\left(\frac{T_s}{T}\right) + \left(\frac{T_s}{T}\right)^{0.5}\left[0.079(1-\chi_{CO_2}-\chi_{O_2}) + 0.106\chi_{CO_2} + 0.036\chi_{O_2}\right]\right\} \qquad (8)$$

$$\bar{\gamma}_{\nu CO_2} = \frac{P}{P_s}\left(\frac{T_s}{T}\right)^{0.7}\{0.07\chi_{CO_2} + 0.058(1-\chi_{CO_2}-\chi_{H_2O}) + 0.1\chi_{H_2O}\},$$

$$\bar{\gamma}_{\nu CO} = \frac{P}{P_s}\left\{0.075\chi_{CO_2}\left(\frac{T_s}{T}\right)^{0.6} + 0.12\chi_{H_2O}\left(\frac{T_s}{T}\right)^{0.82} + 0.06\left(\frac{T_s}{T}\right)^{0.7}(1-\chi_{CO_2}-\chi_{H_2O})\right\} \qquad (10)$$

In these equations, P_s=1 atm, T_s=296 K and T refers to the gas temperature.

The NBS gas parameters $\overline{k_\nu}$ (mean line-intensity to spacing ratio) and $\overline{\delta_\nu}$ (equivalent line spacing) used for this study for H_2O, CO_2 and CO are taken from [8]. These parameters are function of the temperature and are tabulated for a set of spectral interval $\Delta\nu = 25$ cm^{-1}. The temperature and spectral range are respectively 300-2900 K and 150-9300 cm^{-1}. For non-homogeneous and non-isothermal absorbing gas column, the CG approximation based on effective band model parameters is used [5]. The method consists in using Eq. 7 with the following quantities $\overline{K_{eq}}$ and $(\bar{\gamma}/\bar{\delta})_{eq}$:

$$\overline{K_{eq}} = \frac{1}{u}\int_0^L \overline{K}\chi p ds\,,\ (\bar{\gamma}/\bar{\delta})_{eq} = \frac{1}{u\overline{K_{eq}}}\int_0^L (\bar{\gamma}/\bar{\delta})\overline{K}\chi p ds \ \text{ and } \ u = \int_0^L \chi p ds$$

Weighted sum of gray gases (WSGG)

The WSGG represents the total emissivity of a real gas as the sum of the weighted emissivities of a number of gray gases [9, 10]:

$$\varepsilon_g(T, L, p) = \sum_{n=1}^{N} a_n\left[1-\exp(-\kappa_{g,n}pL)\right] \qquad (11)$$

where L is the path length and p the partial pressure of the absorbing species. a_n is the weighting factor for the n th gas and may be interpreted as the fraction of blackbody energy in a spectral region in which the absorption coefficient is close to $\kappa_{g,n}$. Using the WSGG approach, the RTE for spatially constant radiative properties lead to resolution of the set of N equations:

$$\frac{dI_n}{ds} = \kappa_{n,g}p(a_n I_b - I_n) \qquad (12)$$

The total intensity, I is then found by adding the solutions of Eq. 12:

$$I = \sum_{n=1}^{N} I_n \qquad (13)$$

In the present study the WSGG parameters are those of Taylor & Foster [9], for mixtures of H_2O-CO_2 and CO_2-H_2O-soot using respectively a one-clear 3-gray gases and a 3-gray gases for temperatures between 1200 K and 2400 K.

RESULTS AND DISCUSSION

The CK approach NBS and WSGG models are applied to different fires and combustion scenarios. Although the CK formulation has a wider range of application than the NBS and WSGG, especially for taking into account the complex in-scattering term in Eq. 4 the analysis is undertaken to assess its accuracy and compare its prediction to the other

models. Since the NBS and WSGG, as formulated, do not include the in-scattering terms, only soot absorption is considered for these models.
The models are tested first on a 80 cm plexiglas (PMMA) pool fire, typical of combustion environments [10]. The two configurations are called E and F in reference [10]. The experimental distribution profiles of the combustion products are given in Figs. 1 and 2 for configuration E and F respectively. Non-homogeneous and non-isothermal mixtures are considered. For configuration E, simulations with the models have been performed for a line-of-sight along the centreline to the surface of the pool fire. For configuration F, calculations through a line-of-sight outward from the pool are considered. The CK gas model, coupled with the integral approach Eq. 5 is applied to both configurations. The path length is divided into 20 grids. Figure 3 presents the results

obtained by applying the CK, NBS, WSGG approaches to the calculation of radiation intensities. The RADCAL results, presented in ref. [10] are obtained by applied the narrow-band model with the data of Ludwig et al. [11]. The CK method provides a total radiance of 0.71 W/cm^{2}sr at the fuel surface (80 cm). This value is close to the 0.72 W/cm^{2}sr provided by RADCAL and reported by Grosshandler [10]. The NBS and WSGG models give fuel surface radiances of 0.72 W/cm^{2}sr and 0.70 W/cm^{2}sr respectively. The CK model provides results close to NBS ones. The results show that the distribution of radiance between 0 to 80 cm can present discrepancies between models. Although RADCAL and NBS are not based on the same band parameters database, RADCAL results reasonably agree with the CK and NBS as well. A relative difference of 17 % is found in the central region between CK and RADCAL. The WSGG model shows the largest discrepancies with the CK, highlighting the inaccuracy of the approach for this type of configuration. Figure 4 presents the models simulation results for configuration F, where the temperature and gases species concentrations differ considerably from configuration E. The total radiance (total intensity) emanating from the PMMA pool fire is presented. The CK solution provides a total radiance of 0.84 W/cm^{2}sr at the end-path (80 cm), close to the 0.85 W/cm^{2}sr obtained with NBS. The RADCAL provides 1.08 W/cm^{2}sr at the same distance (28 % relative difference with CK) while WSGG gives 0.97 W/cm^{2}sr radiance. For this flame structure the results show that RADCAL and WSGG results differ from the CK approach. For the two configurations, the CK method required 20 s on a Sun Ultra 1 Solaris, the NBS 12 s and the WSGG 0.5 s.

For the second fire system to test, radiation transfer in a 750 kW natural gas industrial diffusion flame is considered [12]. The pressure in the combustion chamber is 10^5 Pa and the gases and soot concentrations were obtained by a sampling probe in which combustion products were diluted. Figures 5 and 6 present respectively the transversal structure of the flame at the distances 0.6 and 1.3 m from the burner exit. Radiation intensities were measured by a narrow-angle probe equipped with a total pyrometer radiation pyrometer. A line-of-sight calculation is carried out with the CK, NBS and WSGG models. Figure 7 presents the calculation results for the flame structure of Fig. 5. The CK model provides results very close to the experimental data. The NBS model, based on the experimental parameters of Ref. [8] provides results that are also close to the experimental data. The measurement errors are not specified in [12]. The CK and NBS results are very close for this configuration and a maximum relative difference of 12 % is found between the two models close to the burner surface. As expected, the WSGG predictions show an important difference with the experiment and the CK approach. The

relative difference WSGG-CK is everywhere larger than 55 %, the worst value is found close to the burner surface (130 %). Figure 8

shows the results using the flame profiles in Fig. 6, at 1.3 m from the burner exit. The soot attenuation by absorption is taken into account by different models. The results show the relatively good agreement with experiment provides by the CK model for this other non-homogeneous and non-isothermal configuration. The NBS results are also close the CK ones and the WSGG model provide poor results. The CPU times are similar to those of the PMMA simulation previously presented.

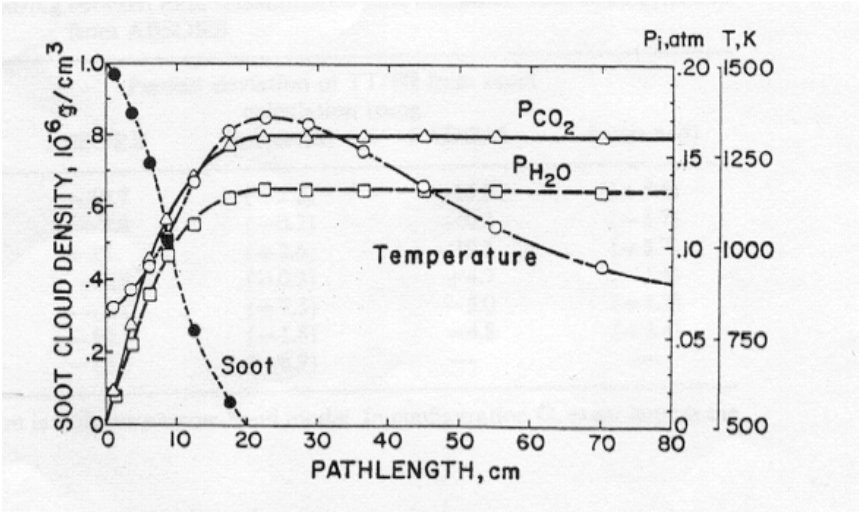

Fig. 1 - Composition and temperature profiles - PMMA pool fire, configuration E [10].

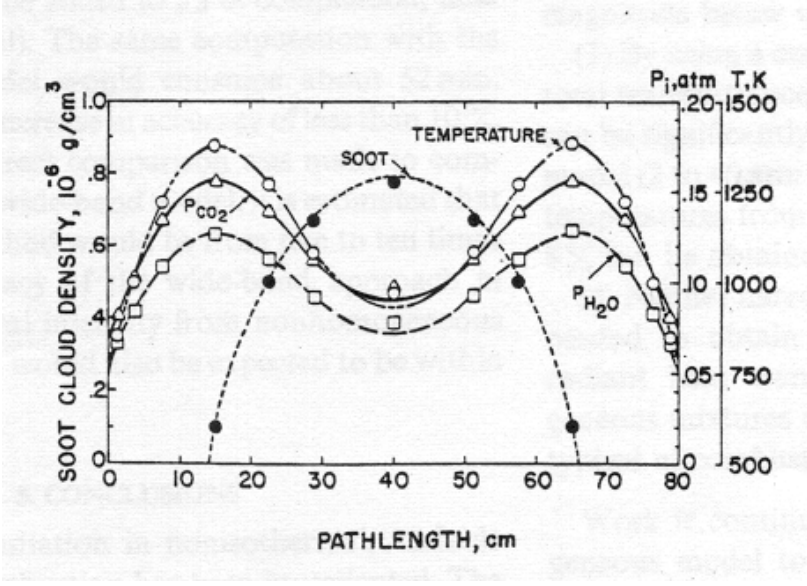

Fig. 2 - Composition and temperature profiles - PMMA pool fire, configuration F [10].

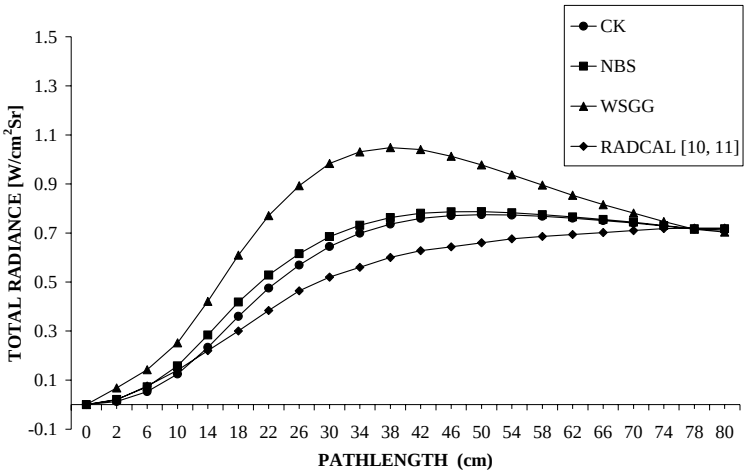

Fig. 3 - Calculated radiance to the surface of a PMMA pool fire, configuration E.

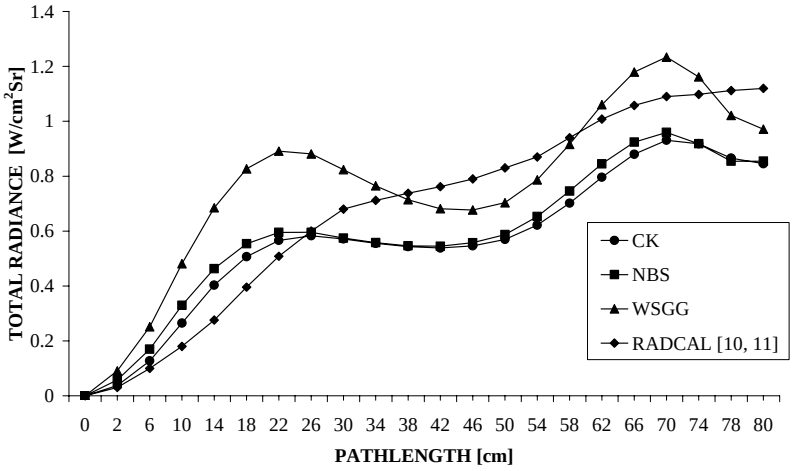

Fig. 4 - Calculated radiance emanating from a PMMA pool fire, configuration F.

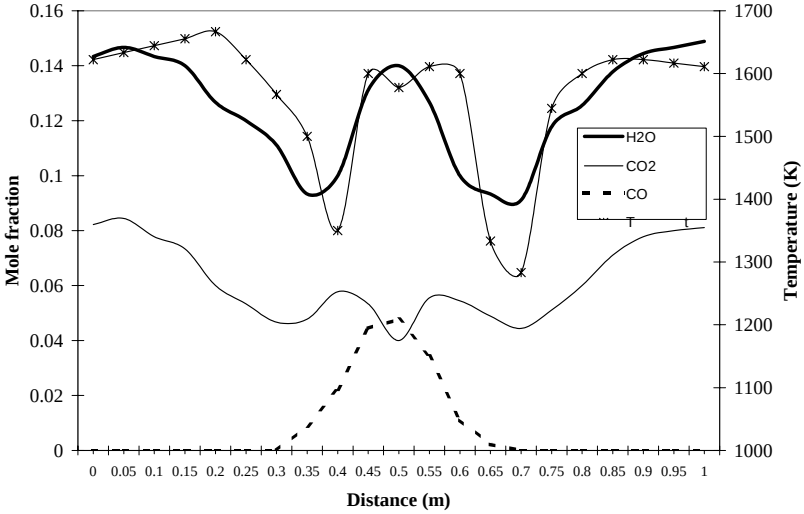

Fig. 5**.** Composition, soot concentration and temperature profiles measured within the natural gas flame at 0.6 m from burner exit – Chamber pressure 10^5 Pa [12].

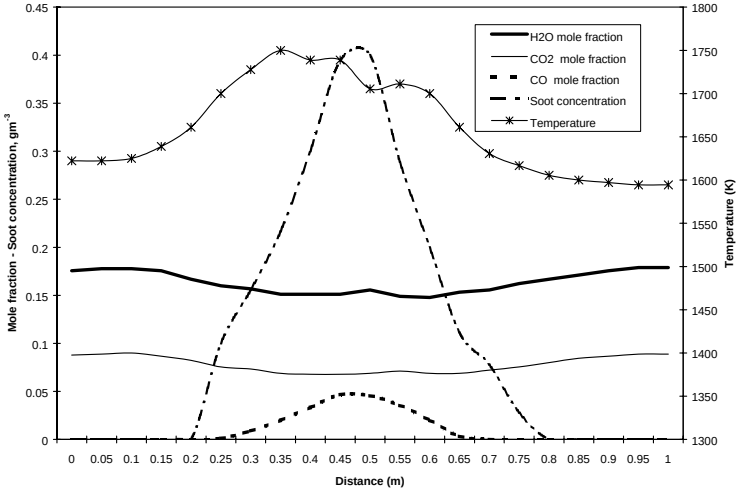

Fig. 6 - Composition, soot concentration and temperature profiles measured within the natural gas flame at 1.3 m from burner exit – Chamber pressure 10^5 Pa [12].

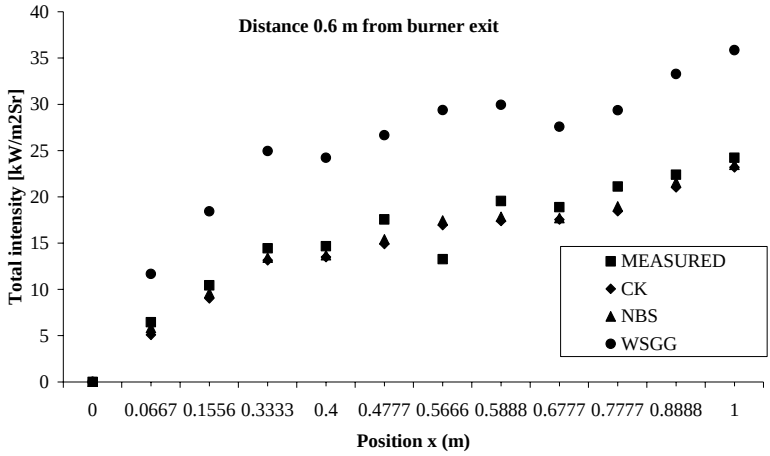

Fig. 7 - Calculated intensity distribution for the flame profile in Figure 5 (0.6 m from burner exit).

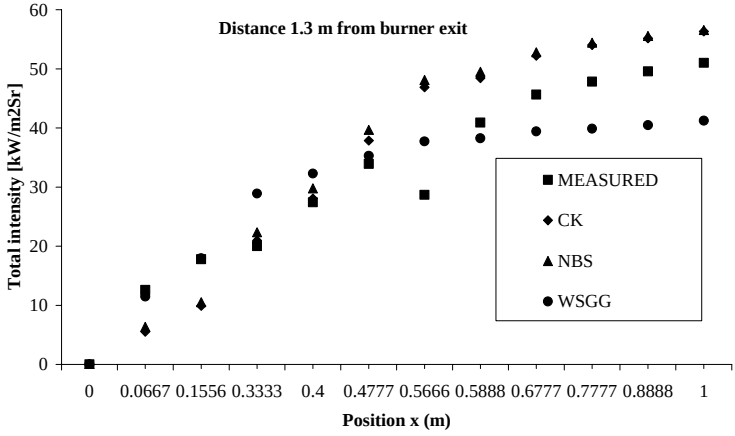

Fig. 8 - Calculated intensity distribution for the flame profile in Figure 6 (1.3 m from burner exit).

CONCLUSIONS

A correlated-k distribution method, based on seven Gaussian quadrature points and a Newton-Raphson procedure for calculation of the re-ordered absorption coefficients $k(g_j)$ has been presented and tested on PMMA and natural gas fires. The spectrally based CK formulation offers the main advantage of being formulated in terms of absorption

coefficient, rather than in transmissivity as NBS models. The model has a wider range of application since it can handle the in-scattering term in the RTE by contrast to NBS. However, when this scaterring term is not accounted for, NBS is the best option. The total radiances or intensities calculations for non-homogeneous and non-isothermal mixtures of gases and soot, typical of PMMA and natural gas fires, have been carried out with CK, NBS and WSGG approach. CK and NBS provide close results when the in-scattering term is not accounted for. The WSGG results by contrast, could present important discrepancies with CK. The results show that the CK formulation, coupled with an integral volume control technique is suitable for combustion systems and could provide good agreement with experiment. These results also prove that, apart from the atmospheric application where it has been extensively used the CK approach can be applied to fire and combustion systems. The CPU times are reasonable for the configurations tested in this study (20 s on a Sun Ultra 1). However, for the implementation of the CK approach in CFD codes, careful attention should be given to the quadrature points $k(g_j)$ calculation in order to speed up the calculations. Instead of a numerical

Newton-Raphson procedure, tabulated values could be generated with an interpolation scheme. This task is the prospect of the current work.

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