

Non-gray Radiation Analysis in Participating Media with the Finite Volume Method

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Abstract

The Weighted-Sum-of-Gray-Gases (WSGG) model is used to investigate radiative heat transfer in non-gray media. The finite volume method (FVM) is used to solve the radiative transfer equation. Validations with benchmarks show satisfactory results when coupling the WSGG model to the FVM. A scattering analysis is then presented where the effects of the scattering albedo and the phase function are studied. Finally, the WSGG model is applied to a gas turbine combustion simulator (GTCS) for prediction of the incident wall radiative heat flux. Comparison of the experimental measurements with the non-gray WSGG numerical results shows satisfactory agreement of the wall radiative heat flux.

Key words: Radiative transfer, FVM, WSGG-model, Non-gray, Scattering.

Introduction

Efficient computation of radiative heat transfer is essential for the design and analysis of industrial thermal systems, such as furnaces, boilers, burners, and gas turbines. In these combustion devices, temperatures are very high and, consequently, thermal radiation plays an important role in the heat transfer mechanisms. Moreover, the radiative properties of combustion products, particularly H_2O and CO_2 , vary strongly and rapidly in wavelength with varying temperature. Consequently, assuming that gray gas has either uniform radiative properties or simple function-of-state variables rather than wavelength may cause significant errors. Hence, including the spectral variation of radiative properties into the radiative heat transfer model is essential for high accuracy.

Several spectral models have been developed to account for the non-gray behavior introduced by the

spectral variation of the combustion products' radiative properties. These models can be grouped into line-by-line (LBL) models, spectral band models, and global models.

The LBL model is the most accurate one to account for radiative properties of gases. In this method, the radiative transfer equation (RTE) is integrated over the detailed molecular spectra of the gases (Ozisik, 1973). However, for combustion applications where the radiative properties of combustion products (mainly H_2O , CO_2 , and soot) vary so strongly and rapidly across the spectrum, many thousands of lines and many thousands of bands are needed (Farias and Carvalho, 1998; Solovjov and Webb, 2005). With this strong spectral variation, the LBL approach becomes computationally expensive and fails to be a practical method for engineering applications. Nevertheless, its exactness makes the model useful for benchmark solutions.

Narrow band models (NBM) are very accurate

and suitable for practical spectral radiation applications (Ludwig et al., 1973). These models require a large number of bands and excessive computing time. Wide band models (WBM) are a simplification of the NBM. They are less accurate, but are more economical, and reasonably accurate (Edwards, 1976). Both NBM and WBM are difficult to be coupled to the solution methods of the RTE, such as the discrete ordinates method (DOM) and the finite volume method (FVM). In fact, the NBM gives the spectral transmissivity averaged over a narrow band, while the WBM yields a wide band absorptivity of a species or a medium. Hence, these models can not easily and simply be incorporated in DOM or FVM, where absorption and extinction coefficients are required. Much research has been oriented to developing models that yield radiative properties based on absorption and scattering coefficients. The correlated-k distribution model (CK) (Goody et al., 1989; Lacis and Oinas, 1991), originally developed for atmospheric radiation and meteorological applications, presents such opportunity. Indeed, in this model, the black-body radiation intensity within a spectral band is constant, and the spectral integration over the wavenumber in a band is replaced by a quadrature over the absorption coefficient. The radiation intensity varies with the absorption coefficient, and is reordered into a smoothly increasing intensity function. With this behavior, it is easier to couple the CK model with DOM or FVM solution methods of the RTE than with NBM and WBM. Due to this advantage, the CK model received the attention of many researchers and gave rise to hybrid models.

Global models are based on the concept of the Weighted Sum of Gray Gases Model (WSGG). It was first presented by Hottel and Sarofim (1967) and it has been the most widely used global model for the calculation of gas radiative properties. In this model, the radiative properties of real gases (non-gray gas) are replaced with an equivalent finite number of gray gases. When using this model, the RTE is solved for each gray gas and the total heat flux is obtained by adding the heat flux of the gray gases after multiplication with certain weight factors (Modest, 1991). Coelho (2002) applied the WSGG model in a 3-D enclosure and compared it with the CK model. Trivic (2004) coupled the WSGG to the FVM to study non-gray radiation in 3-D enclosures. Yu et al. (2000) extended the model to a two-phase mixture of non-gray gases with particles. Yang and Song (1999) used a hybrid model, WSGG-based narrow band for CO₂

at 4.3 μm . Kim and Song (2000) applied the WSGG-based spectral model and presented databases for radiative properties of combustion gases.

In this paper, the WSGG model is coupled to the FVM. Three non-gray benchmark test cases of pure water vapor media, at uniform temperature, are used for validation. In the first 2 cases, the H₂O concentration profile is uniform in the medium, while in the third case, the water vapor has a parabolic concentration profile. Comparison with benchmarks shows that the WSGG results are satisfactory. Then a scattering analysis featuring the effects of the scattering phase function and the scattering albedo on the radiative source term and the radiative heat flux is presented. In the last part of this work, the WSGG is used to study the radiative transfer in a gas turbine combustion simulator (GTCS) that was experimentally documented. Compared to the gray case, the non-gray results of the simulation featured more satisfactory agreement with the experimental measurements.

Radiation model description

Radiative transfer equation The derivation of the RTE, the significance of each term, and all the details are presented in the literature (Siegel and Howell, 1981; Modest, 2003). In a participating medium, the spectral RTE can be written as

$$\begin{aligned} \frac{dI_\lambda(\vec{s}, \vec{r})}{ds} = & -(\kappa_\lambda + \sigma_{s\lambda})I_\lambda(\vec{s}, \vec{r}) + \kappa_\lambda I_{b\lambda}(\vec{r}) \\ & + \frac{\sigma_{s\lambda}}{4\pi} \int_{\Omega'=4\pi} \Phi_\lambda(\vec{s}', \vec{s}) I_\lambda(\vec{s}', \vec{r}) d\Omega' \end{aligned} \quad (1)$$

where I_λ is the spectral radiation intensity, I_b is the black body radiation intensity, and κ_λ and $\sigma_{s\lambda}$ are the spectral absorption and scattering coefficients, respectively. $\Phi(\vec{s}', \vec{s})$ is the scattering phase function, which describes the probability that a ray from one direction \vec{s}' will be scattered into the direction \vec{s} .

The boundary condition for a diffusely emitting and reflecting wall is

$$\begin{aligned} I(\vec{s}, \vec{r}_w) = & \varepsilon_w I_{b,w}(T_w) \\ & + \frac{1 - \varepsilon_w}{\pi} \int_{\vec{s}' \cdot \vec{n}_w < 0} I(\vec{s}', \vec{r}_w) |\vec{s}' \cdot \vec{n}_w| d\Omega' \end{aligned} \quad (2)$$

This last equation indicates that the leaving intensity at the wall is the sum of the emitted and the reflected intensities.

The net and incident radiative heat fluxes are written as

$$q_\lambda = \int_{\Omega=4\pi} I_\lambda(\vec{s}, \vec{r}) \cdot (\vec{s} \cdot \vec{n}) d\Omega \quad (3)$$

$$G_\lambda = \int_{\Omega=4\pi} I_\lambda(\vec{s}, \vec{r}) d\Omega \quad (4)$$

The divergence of the radiative heat flux from the medium is given by

$$\nabla \cdot q_\lambda = \kappa_\lambda (4\pi I_{b\lambda} - G_\lambda) \quad (5)$$

Since the radiative intensity is a function of position and direction, both spatial and directional discretizations are needed. The FVM is well suited for this type of problem (Raithby and Chui, 1990; Chai et al., 1994; Kim and Baek, 1997). In this method, the solution domain is first subdivided into discrete, non-overlapping control volumes ΔV , each of which contains at its center a node P. At each node, the direction is subdivided into non-overlapping discrete solid angles $\Delta\Omega^m$, which always sum up to 4π steradians. The RTE is then integrated over a control volume ΔV and a control angle $\Delta\Omega^m$. The final discretized form of the RTE is expressed in the cylindrical coordinate system and is written as (the spectral dependency is omitted for clarity of the equations)

$$a_P^m I_P^m = \sum_{J=E,W,S,N} a_J^m I_J^m - \frac{\Delta V}{r} \alpha^{m-\frac{1}{2}} I_P^{m-1} + S_{\text{mod}}^m \Delta V \Delta\Omega^m \quad (6)$$

$$a_J^m = -\Delta A_i D_{i,in}^m \quad (7)$$

$$a_P^m = \sum_i \Delta A_i D_{i,out}^m - \frac{\Delta V}{r} \alpha^{m+\frac{1}{2}} + \beta_{\text{mod}} \Delta V \Delta\Omega^m \quad (8)$$

$$\beta_{\text{mod}} = \beta - \frac{\sigma_s}{4\pi} \Phi_{m \rightarrow m} \Delta\Omega^m \quad (9)$$

$$S_{\text{mod}}^m = \kappa I_b + \frac{\sigma_s}{4\pi} \sum_{m' \neq m}^M I^{m'} \bar{\Phi}_{m' \rightarrow m} \Delta\Omega^{m'} \quad (10)$$

where $D_i^m = \int_{\Delta\Omega^m} (\vec{s} \cdot \vec{n}_i) d\Omega$ are the directional weights.

$\bar{\Phi}_{m \rightarrow m'}$ denotes the scattering phase function and $\bar{\Phi}$ is its averaged value and is expressed as

$$\bar{\Phi}_{m' \rightarrow m} = \frac{\int_{\Delta\Omega^m} \int_{\Delta\Omega^{m'}} \Phi(\vec{s}', \vec{s}) d\Omega' d\Omega}{\Delta\Omega^m \Delta\Omega^{m'}} \quad (11)$$

while the boundary condition is discretized as

$$I_w^m = \varepsilon_w I_{b,w}(T_w) + \frac{1 - \varepsilon_w}{\pi} \sum_{\vec{s}' \cdot \vec{n}_w < 0} I_w^{m'} \left| D_{w,in}^{m'} \right| \quad \text{for } \vec{s} \cdot \vec{n}_w > 0 \quad (12)$$

The WSGG model The WSGG approach was first introduced by Hottel and Sarofim (1967). In this model, the non-gray gas is replaced by a number of gray gases for which the radiative heat transfer rates are calculated independently. The total heat flux is then found by adding the heat fluxes of the gray gases after multiplication with certain weight factors. However, the total gas emissivity is approximated by a summation of a number of terms, each one being the multiplication of a weighting factor and a gray emissivity. The total emissivity and absorptivity are evaluated from the following equations:

$$\varepsilon = \sum_i^{Ng} a_{\varepsilon,i}(T) [1 - e^{-\kappa_i PS}] \quad (13)$$

$$\alpha = \sum_i^{Ng} a_{\alpha,i}(T, T_w) [1 - e^{-\kappa_i PS}] \quad (14)$$

where $a_{\varepsilon,i}$, $a_{\alpha,i}$, and κ_i are the weighting factors and the absorption coefficient of the i^{th} gray gas, respectively. Their values are obtained by fitting Eq. (12) and Eq. (13) to total emissivity and absorptivity (Truelove, 1976; Smith et al., 1982). The weighting factors may be a function of temperature. Smith et al. (1982) used third-order polynomials for both

$a_{\varepsilon,i}$ and $a_{\alpha,i}$. For an H₂O-CO₂-N₂ mixture at atmospheric pressure P , and with $P_{H_2O} = 0.2P$ and $P_{CO_2} = 0.1P$, Truelove (1976) employed linear expressions. Physically, these coefficients may be interpreted as the fractional amounts of black body energy in the spectral region where a gray gas having absorption coefficient κ_i exists. For a transparent region of the spectrum (clear gas), the absorption coefficient is set to zero in order to account for windows in the spectrum between spectral regions of high absorptions.

The weighting factors must sum to unity and be positive. For the clear gas, the weighting factors are evaluated from the following relations

$$a_{\varepsilon,0} = 1 - \sum_{i=1}^{Ng} a_{\varepsilon,i} \quad (15)$$

$$a_{\alpha,0} = 1 - \sum_{i=1}^{Ng} a_{\alpha,i} \quad (16)$$

Using the WSGG model, the RTE for the i^{th} gray gas may be expressed as

$$\begin{aligned} \frac{dI_i(\vec{s}, \vec{r})}{ds} = & -(\kappa_i + \sigma_s)I_i(\vec{s}, \vec{r}) + \kappa_i I_{b,i}(\vec{r})a_i(T) \\ & + \frac{\sigma_s}{4\pi} \int_{\Omega'=4\pi} \Phi(\vec{s}', \vec{s}) I_i(\vec{s}', \vec{r}) d\Omega' \end{aligned} \quad (17)$$

subject to the boundary condition

$$\begin{aligned} I_i(\vec{s}, \vec{r}_w) = & \varepsilon_w I_{b,w}(T_w)a_i(T) \\ & + \frac{1 - \varepsilon_w}{\pi} \int_{\vec{s}' \cdot \vec{n}_w < 0} I_i(\vec{s}', \vec{r}_w) |\vec{s}' \cdot \vec{n}_w| d\Omega' \end{aligned} \quad (18)$$

After solving the RTE for each gray gas, the total radiation intensity, the incident heat flux, the net heat flux, and the radiative source term are respectively calculated from the following relations

$$I^m = \sum_{i=0}^{Ng} I_i^m \quad (19)$$

$$G_{tot}(\vec{r}) = \sum_{i=1}^{Ng} G_i(\vec{r}) = \sum_{i=1}^{Ng} \int I_i(\vec{r}, \vec{s}) d\Omega \quad (20)$$

$$q_{\vec{n}_k, tot}(\vec{r}) = \sum_{i=1}^{Ng} q_{\vec{n}_k, i}(\vec{r}) = \sum_{i=1}^{Ng} \int I_i(\vec{r}, \vec{s}) (\vec{s} \cdot \vec{n}_k) d\Omega \quad (21)$$

$$\nabla \cdot q_{tot}(\vec{r}) = \sum_{i=1}^{Ng} \nabla \cdot q_i(\vec{r}) = \sum_{i=1}^{Ng} \kappa_i [4\pi a_i(T)I_b(\vec{r}) - G_i(\vec{r})] \quad (22)$$

Description of the test cases

Four radiative heat transfer problems are described in the following sections. The first three are 1D cases, which are used to validate the numerical tool, while the fourth is a 2D case study. In the first test case, a pure H₂O vapor at atmospheric pressure is considered at a uniform temperature of 1000 K. The medium is bordered by 2 infinite parallel plates, which are black and cold, and separated by a distance $L = 0.1$ m. The second test case is similar to the first, under the same conditions; the only difference is that the medium is considered thick, with a separation distance between the plates of $L = 1.0$ m. However, in the third test case, the medium has a uniform temperature $T = 1000$ K and a path length $L = 1.0$ m, while the water vapor has a parabolic concentration profile ($X_{H_2O} = 1 - 4 \times (z - 1/2)^2$). In all cases the slab is divided into 20 sub-layers and the FVM is used with an angular discretization of $(N_\theta \times N_\psi) = (8 \times 12)$. The WSGG model predictions are compared to those obtained by Kim et al. (1991) with the NBM.

In the fourth test case, a GTCS is considered. The GTCS presents the advantages of being a real test case providing input data and measurements of the incident wall radiative heat flux, which can be compared to the computational predictions. As described by Kayakol (1998) and Kayakol et al. (2000), the GTCS is a cylindrical enclosure fired with a turbulent diffusion flame of propane with air. The combustion chamber has a length of 420 mm and a diameter of 101.6 mm. The temperature and the H₂O/CO₂ mixture composition are listed elsewhere

(Kayakol, 1998). In this experimental test case, non-gray analysis is accomplished by the WSGG model, and the FVM is used as the solution method of the RTE. Non-gray predictions of the incident radiative heat flux at the side wall of the combustor are compared to those obtained with global radiative properties.

Results and Discussion

Isothermal medium with a uniform H₂O concentration profile

For the first two test cases, the medium contains 100% H₂O at atmospheric pressure. The WSGG model is coupled to the FVM in order to predict the net wall heat flux and the radiative source term. The WSGG model is used with 4 gray gases ($N_g = 3 + 1$ clear gas) where the weighting coefficients and the radiative properties are reported by Smith et al. (1982). Results for the net wall heat fluxes are reported in Table 1 and compared with those predicted by the NBM of Kim et al. (1991). Comparison of the radiative source term predictions shows a good agreement between the WSGG results and the mentioned reference. This is confirmed by Figures 1(a) and 1(b), where the divergence of the radiative heat fluxes is reported.

Table 1. Net radiative heat flux at the wall (kW/m²).

Test Cases	Kim et al. (1991)	WSGG
L = 0.1 m	14.3	14.53
L = 1.0 m	28.2	26.60
Parabolic profile of H ₂ O	25.4	24.63

The scattering effect is described with 4 phase functions, which are the forward F1 and F3, the isotropic, and the backward B2 functions, as described by Kim and Lee (1988). The net wall radiative heat fluxes are computed for a scattering albedo $\omega = 0.7$ and are reported in Table 2. The results show that the scattering phenomenon decreases the net heat flux. With reference to isotropic scattering, the results also show that the forward F1 and F3 functions enhance radiative transfer near the walls, while the backward B2 function decreases this transfer.

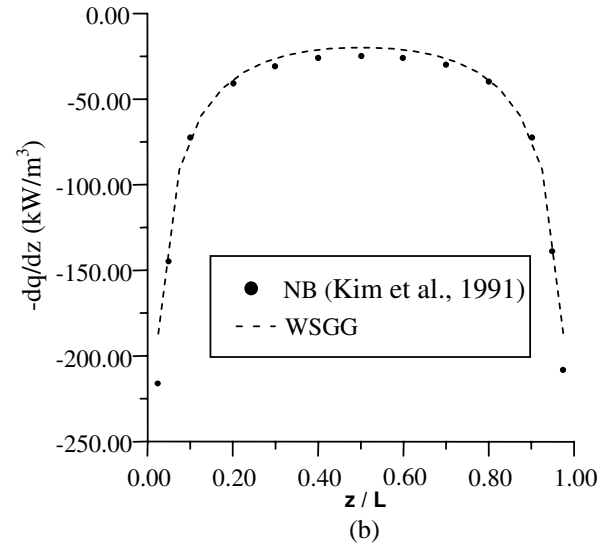
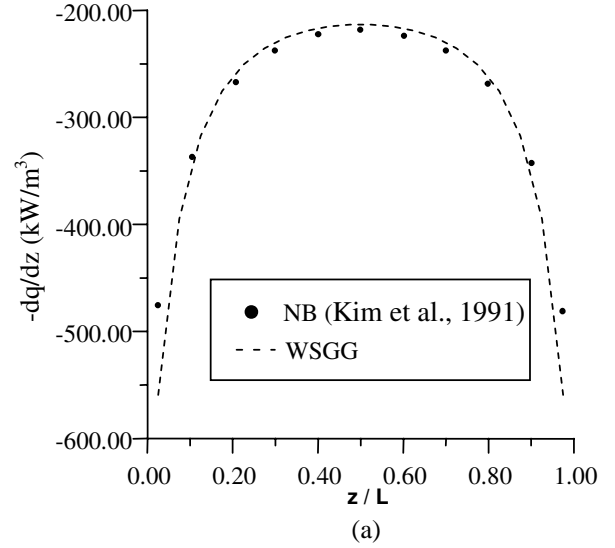


Figure 1. Radiative source term: (a) L = 0.1 m, (b) L = 1.0 m.

Table 2. Effect of the scattering phase function on the net wall heat flux (kW/m²).

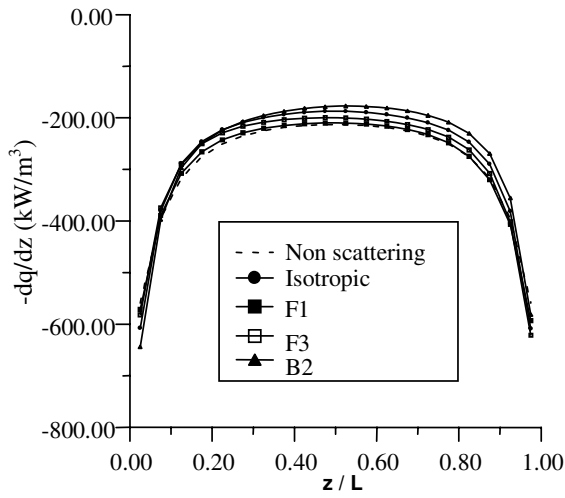
Scattering phase function ($\omega = 0.7$)	Test cases	
	Case 1 L = 0.1 m	Case 2 L = 1.0 m
Non scattering	14.5305	26.6031
F1	14.4444	25.8273
F3	13.8141	24.2919
Isotropic	13.4965	23.7344
B2	13.4375	23.6471

Moreover, Figures 2(a) and 2(b) show that the scattering phenomenon decreases the radiative source term in the medium and makes its distribution more uniform. The figures also show that scattering affects the radiative transfer in the thin medium more than in the thick medium. Similar remarks can be reproduced when analyzing the scattering albedo effect as shown in Figures 3(a) and 3(b), and Table 3. Indeed, increasing the scattering albedo ω decreases the net radiative heat flux and the radiative source term. This is due to the uniformity produced by the scattering phenomenon in the medium. Moreover, greater effect of the scattering

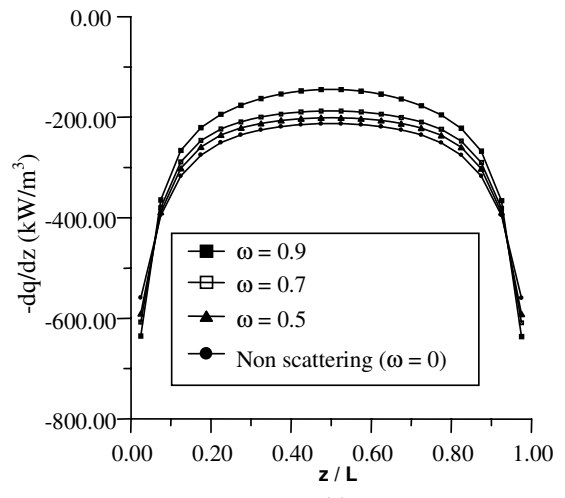
albedo is observed for the thin medium than for the thick one.

Table 3. Effect of the scattering albedo on the net wall heat flux (kW/m^2).

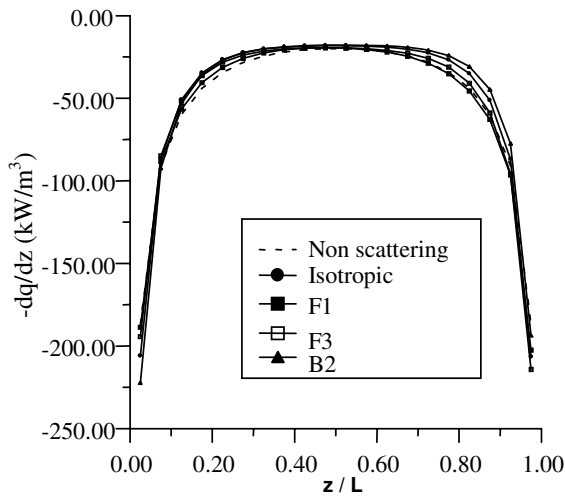
Scattering Albedo (Isotropic scattering)	Test cases	
	Case 1 L = 0.1 m	Case 2 L = 1.0 m
$\omega = 0.0$	14.5305	26.6031
$\omega = 0.5$	14.0450	24.8821
$\omega = 0.7$	13.4965	23.7350
$\omega = 0.9$	11.7187	21.4188



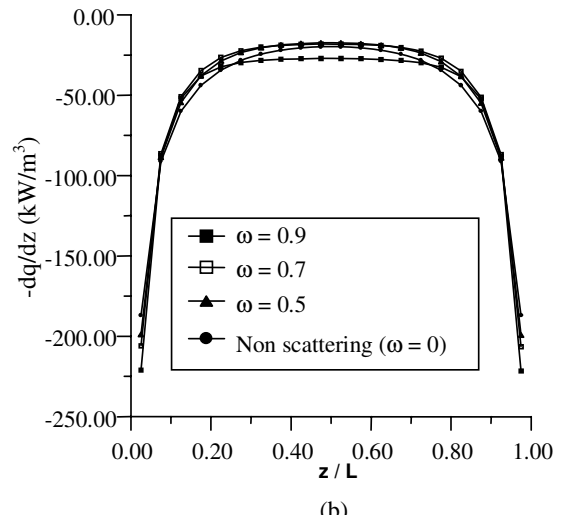
(a)



(a)



(b)



(b)

Figure 2. Effect of the scattering phase function: (a) L = 0.1 m, (b) L = 1.0 m.

Figure 3. Effect of the scattering albedo: (a) L = 0.1 m, (b) L = 1.0 m.

Isothermal medium with parabolic H_2O concentration profile

For the parabolic concentration profile of H_2O , the predictions of the radiative source term are reported in Figure 4 and the wall radiative heat flux is already given in Table 1. The results are compared to those obtained by the NBM of Kim et al. (1991) and to the LBL benchmark of Ludwig et al. (1973). Comparison shows that the WSGG model over-predicts the radiative source term inside the medium, while acceptable results for the heat flux are obtained. In fact, the WSGG is used with only 4 gray gases (3 + 1 clear gas), and on the computational time basis it is a very attractive model. Hence, a compromise between accuracy and computational time arises. However, the WSGG predictions present similar trends with the benchmarks.

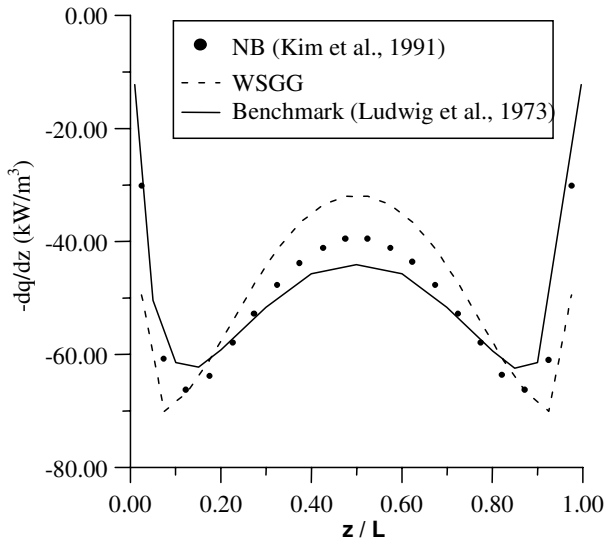


Figure 4. Radiative source term for a parabolic concentration profile of H_2O .

Gas turbine combustion simulator

In the fourth test case, radiative heat transfer in the GTCS is analyzed with the non-gray WSGG model. The 2 different expressions of the weighting coefficients, given by Smith et al. (1982) and Truelove (1976) are used. The GTCS medium contains an H_2O/CO_2 mixture. The concentration profile of each component is reported by Kayakol (1998). From these profiles, the X_{H_2O}/X_{CO_2} ratio is near 2. Consequently, the weighting coefficients of Smith

et al. (1982) correspond to $P_{H_2O}/P_{CO_2}=2$, while the ones used by Truelove (1976) are those of a 20% H_2O / 10% CO_2 / 70% N_2 mixture. For both expressions, the incident radiative heat fluxes at the side wall are compared and shown in Figures 5(a) and 5(b). The FVM is used with 2 angular discretization grids, $(N_\theta \times N_\psi) = (6 \times 8)$ and $(N_\theta \times N_\psi) = (8 \times 10)$.

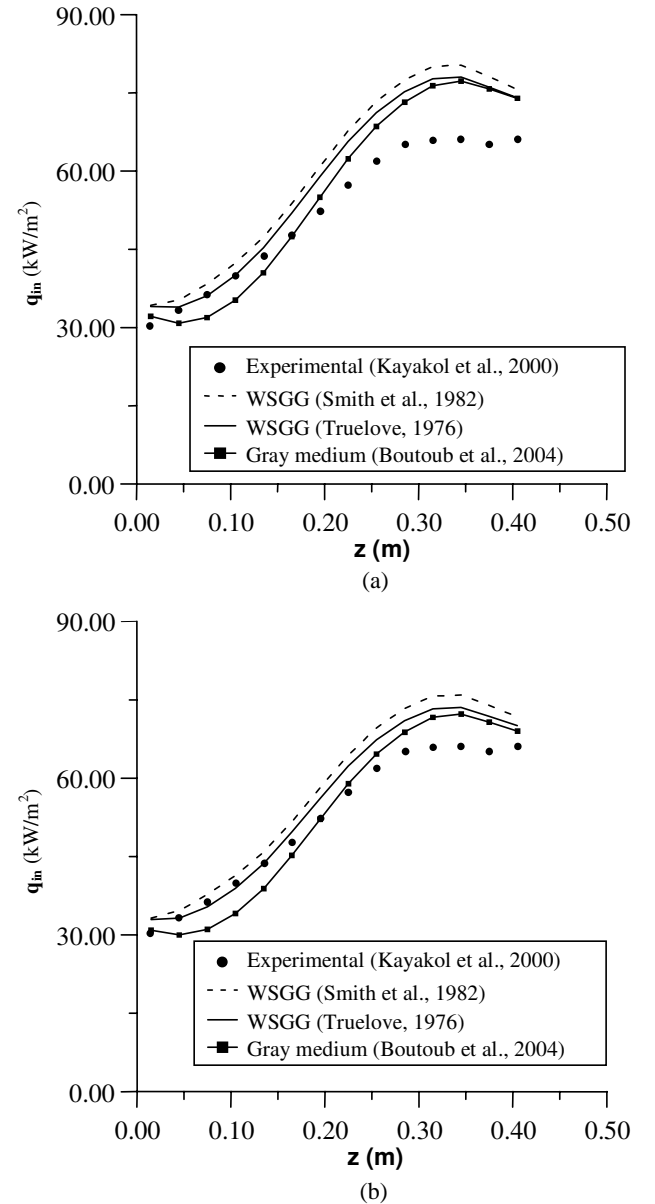


Figure 5. Incident radiative heat flux at the side wall of the GTCS (a) FVM (6×8) , (b) FVM (8×10) .

Analysis of the 2 figures shows that for the GTCS application, the coefficients of Smith et al. (1982) give slightly higher values in comparison with the experimental measurements than the coefficients of Truelove (1976). Predictions with the gray medium assumption are also reported in Figure 5 (Boutoub et al., 2004). Comparison with the experimental data shows better agreement of the non-gray predictions, especially in the first half of the GTCS. Moreover, Figure 5(b) shows that much better agreement is obtained when the FVM angular discretization is refined to $(N_\theta \times N_\psi) = (8 \times 10)$. For this experimental test case, Kayakol et al. (2000) showed that the uncertainty in the thermocouple measurements is about $\pm 5\%$ for the gas temperature and is about $\pm 2\%$ for the wall temperature; while for the heat flux measurements, the uncertainty is $\pm 7\%$. Hence, the observed discrepancy between the computational predictions and the experimental data could be due to temperature and incident wall radiative heat flux measurement uncertainties.

Conclusion

The WSGG non-gray radiation model, which is based on the absorption coefficient in the medium is used to study 4 different cases of radiative heat transfer. The FVM is used as the solution method of the radiative transfer equation. The WSGG model, used with 4 gray gases (3 + 1 clear gas), gives satisfactory results. It also proved to be a very economical model even though a compromise between accuracy and computational time arises. A scattering analysis is then presented and the results show that the scattering phenomenon decreases the net heat flux and that, with reference to isotropic scattering, the forward F1 and F3 functions enhance radiative transfer near the walls, while the backward B2 function decreases this transfer. Moreover, more uniformity of the radiative source term is observed when introducing the scattering phenomenon, especially when the medium is thin. In the last part of this work, a case study of radiative heat transfer in a GTCS is analyzed with the non-gray WSGG model. Two different expressions of the weight factors are used. Results show that the non-gray predictions are satisfactory when compared to the experimental data.

Nomenclature

$a_{\varepsilon,i}$	emissivity weighting factors
$a_{\alpha,i}$	absorptivity weighting factors
D_i^m	directional weight
G	total incident radiation
I	radiation intensity
N_g	number of gray gases
\vec{n}_i	unit normal vector at the control volume face i
P	pressure
q	radiative heat flux
r, z	cylindrical coordinates
\vec{r}	position vector
s	distance traveled by a ray
\vec{s}	unit directional vector
T	temperature
X	molar or volume fraction
$\alpha^{m\pm 1/2}$	coefficients of the angular derivative term
β	extinction coefficient
ΔA	surface area of the control volume faces
ΔV	control volume
$\Delta\Omega$	control angle
ε	emissivity
Φ	scattering phase function
κ	absorption coefficient
λ	wavelength
θ, ϕ	polar and azimuthal angles
σ	Stefan-Boltzmann constant
σ_s	scattering coefficient
τ	transmissivity
ω	scattering albedo

Subscripts

b	black body
i	control volume faces (east, west, north, south)
in	incoming
J	neighbors of the node P (East, West, North, South)
out	outgoing
w	wall

Superscripts

m, m'	radiation direction
+, -	boundaries of the control angle

Abbreviations

CK	correlated-k distribution
DOM	discrete ordinates method
FVM	finite volume method

LBL	line by line
NBM	narrow band model
WBM	wide band model
WSGG	weighted sum of gray gases

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