International Journal of Heat and Mass Transfer 124 (2018) 475–483

Contents lists available at ScienceDirect

International Journal of Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ijhmt

Evaluation of the WSGG model against line-by-line calculation of thermal radiation in a non-gray sooting medium representing an axisymmetric laminar jet flame

Felipe R. Centeno [a,*], Rogério Brittes [b], Luís G.P. Rodrigues [a], Felipe R. Coelho [a], Francis H.R. França [a]

[a] Federal University of Rio Grande do Sul, Department of Mechanical Engineering, Porto Alegre, RS, Brazil
[b] Federal University of Santa Maria, Cachoeira do Sul, RS, Brazil

ARTICLE INFO

Article history:
Received 15 November 2017
Received in revised form 15 January 2018
Accepted 10 February 2018

Keywords:
Radiative heat transfer
Sooting flame
LBL integration
WSGG model

ABSTRACT

This paper presents an evaluation of the weighted-sum-of-gray-gases (WSGG) model in the computation of the radiative heat transfer in an axisymmetric gas system composed of H_2O, CO_2 and soot by comparison with line-by-line (LBL) integration. The test cases consider temperature and species concentrations fields that are representative of a laminar diffusion jet flame of ethylene diluted with H_2O. Different approaches are considered in the application of the WSGG model, including the use of WSGG coefficients obtained for different ratios between the mole concentrations of H_2O and CO_2, and the superposition between the coefficients of H_2O/CO_2 and soot. The WSGG coefficients for H_2O and CO_2 are based on HITEMP2010 database, while for soot they are based on the consideration of linear spectral dependence of its absorption coefficient. The spatial integration of the radiative transfer equation is carried out with the discrete ordinates method. The results in the paper show that, although the ratio between the mole concentrations of H_2O and CO_2 varies locally in the flame, using WSGG coefficients for a constant ratio, but equivalent to the global average ratio in the flame, can provide satisfactory solutions in comparison to the LBL integration. Moreover, the superposition method between the WSGG coefficients of combined H_2O/CO_2 and of soot proved accurate considering both moderate and high concentrations of soot. The paper provides algebraic relations for the temperature and concentration fields, which can be used for the evaluation of other gas models in future studies.

1. Introduction

Thermal radiation is generally the main heat transfer mechanism in combustion processes, due to the formation of participating species, such as H_2O, CO_2 and soot, at high temperatures. Possibly the main challenge in computing the radiative transfer is accounting for the complex dependence of the spectral absorption coefficient with the wavenumber. For gases such as H_2O and CO_2, the spectrum involves millions of transition lines. Another difficulty is accounting for variations in the mole concentrations of the participating species in the flame. For instance, soot is often contained in a limited portion of the flame, and the ratio between the mole concentrations of the gaseous species can vary locally due to their different diffusion rates.

Line-by-line (LBL) calculations can deal with local variations in the concentration of the participating species by direct combination of the spectral coefficient of the different species, but the integration over the entire spectrum can be excessively costly for the majority of engineering applications. Global gas models, which cover the entire wavenumber spectrum, require only a fraction of the computational effort of LBL solutions, but strong variations in the local thermodynamic state (temperature and concentration fields) is still a challenge. Thus, there has been a continuous effort in the improvement of the models. Some of the latest developments and reviews of global gas models based on k-distributions can be found in [1–6]. One particular aspect of k-distributions methods is that it normally requires the establishment of a reference thermodynamic state when solving non-uniform media, which can become more critical in presence of steep variations in the thermodynamic state, as it happens in flames. In [5] and [6], a formulation that avoids the use of the reference state was proposed in the framework of the SLW and FSK methods, but it was presented only in terms of variations in the temperature. The weighted-sum-of-gray-gases (WSGG) model does not make use of a reference state, since the correlations of the model are

* Corresponding author.
E-mail address: frcenteno@mecanica.ufrgs.br (F.R. Centeno).

https://doi.org/10.1016/j.ijheatmasstransfer.2018.02.040
0017-9310/

Nomenclature

a	WSGG temperature dependent coefficient, dimensionless
b	polynomial coefficients of the WSGG model, dimensionless
f_v	soot volumetric fraction, dimensionless
I_η	spectral radiation intensity, W/(m^2·cm^{-1}·sr)
I_j	j-th partial radiation intensity, W/(m^2·sr)
p_χ	partial pressure of absorbing species χ, atm
p_T	total pressure of the gas mixture, atm
q_{rad}	radiative heat flux, W/(m^2)
S_{rad}	radiative heat source, W/(m^3)
T	temperature, K
Y_χ	mole concentration of absorbing species χ, dimensionless

Greek symbols

β	fuel dependent soot constant, dimensionless
γ	deviation between the WSGG and the LBL solutions, %
ζ	dimensionless axial position, dimensionless
$\kappa_{\chi,j}$	j-th gray gas absorption coefficient of species χ, m^{-1}
κ_η	spectral absorption coefficient, m^{-1}
κ_p	pressure absorption coefficient, m^{-1}·atm^{-1}
κ_{fv}	volumetric fraction absorption coefficient, m^{-1}
μ	discrete ordinates method direction, dimensionless
ξ	discrete ordinates method direction, dimensionless
ρ	dimensionless radial position, dimensionless
σ	Stefan-Boltzmann constant, 5.670×10^{-8} W/(m^2·K^4)
ξ	discrete ordinates method direction, dimensionless

Subscripts

b	blackbody
c	carbon dioxide
j	j-th WSGG model gray gas
m	mixture
s	soot
w	water vapor
η	spectral dependency

Abbreviations

FSK	full spectrum k-model
LBL	line-by-line integration
RTE	radiative transfer equation
SLW	spectral line based weighted-sum-of-gray-gases model
WSGG	weighted-sum-of-gray-gases model

obtained from a global fitting of gas emittance data, but the model relies on other simplifications such as the consideration of fixed ratios between the mole concentrations of H_2O and CO_2 [7–14]. In one alternative approach [15], the WSGG correlations were obtained separately for H_2O, CO_2 and soot; then a superposition method was applied to solve problems in which their relative concentrations varied from point to point. Evaluations of gas models against LBL solutions are usually presented for one-dimensional slabs, as in most of the above references. Two-dimensional systems are considered in [16–18], but since the temperature and concentration fields cannot be directly recovered, their LBL results cannot be easily used to evaluate other gas models. In [19], a LBL solution of a 2D enclosure with explicit correlations for the temperature and H_2O/CO_2 concentration fields was presented, but soot was not considered.

The present paper presents a study on the accuracy of the WSGG model in the solution of the radiative transfer in a 2D axisymmetric medium representing an ethylene-air laminar diffusion jet flame with soot formation. The temperature and concentration fields of the participating species are presented in terms of algebraic correlations that fit data generated from a global simulation of the flame. The correlations provided in this study can be used to test other gas models. In the present test cases, it is considered that ethylene fuel is diluted with H_2O vapor (50% in volume). It follows from this that, on a global basis, the mole concentration ratio of H_2O and CO_2 in the flue gas is $Y_w/Y_c = 1.5$, but in the flame the ratio is not locally uniform. Different approaches are used for the application of the WSGG model with regard to the H_2O/CO_2 mixture, including the combination of results obtained for uniform concentration ratios of $Y_w/Y_c = 1$ and 2 [7], the superposition method between coefficients of pure H_2O and CO_2 [15], and using newly obtained WSGG coefficients for $Y_w/Y_c = 1.5$. Soot is combined with H_2O/CO_2 radiation by means of the superposition method [15]. The WSGG coefficients for H_2O and CO_2 as well as the LBL integration are based on the HITEMP2010 database [20]. The spatial integration of the radiative transfer equation is accomplished with the discrete ordinates method with S6 quadrature [21]. For laminar flow conditions, the radiation heat transfer is not affected by turbulence-radiation interactions, which simplifies the evaluation of gas models. At the same time, the steep variations in the temperature and concentration fields make this a challenging problem for the evaluation of gas models.

2. Radiative transfer equation in cylindrical coordinates

The radiative transfer equation (RTE) establishes a relation for the variation of the spectral radiation intensity I_η along a certain path in the medium. In the framework of the discrete ordinates method and cylindrical coordinates, the RTE for non-scattering media is given by:

$$\frac{\partial I_\eta}{\partial s} = \mu\frac{\partial I_\eta}{\partial r} + \xi\frac{\partial I_\eta}{\partial z} - \frac{\varsigma}{r}\frac{\partial I_\eta}{\partial \varphi} = -\kappa_{\eta,m} I_\eta + \kappa_{\eta,m} I_{\eta b} \tag{1}$$

where μ, ς, and ξ are the directions, η is the wavenumber, $I_{\eta b}$ is the blackbody spectral intensity evaluated at local conditions, and $\kappa_{\eta,m}$ is the spectral absorption coefficient of the medium. The above equation considers only absorption and emission in the medium, since scattering effects in soot are of minor significance under the conditions of the present study [22,23]. In Eq. (1), the index m appears in $.\kappa_{\eta,m}.$ to consider that the medium can be formed by a mixture of H_2O, CO_2 and soot. In this case, it corresponds to:

$$\kappa_{\eta,m} = \kappa_{\eta,w} + \kappa_{\eta,c} + \kappa_{\eta,s} \tag{2}$$

where the subscripts w, c and s stand for H_2O, CO_2 and soot, respectively. The spectral absorption coefficients, $\kappa_{\eta,w}$, $\kappa_{\eta,c}$, and $\kappa_{\eta,s}$, can vary along the path due to variations in the local temperature and/or concentrations of the participating species.

Once the RTE is solved, the divergence of the radiative heat flux $\nabla \cdot \vec{q}_r$ is calculated as:

$$S_{rad} = -\nabla \cdot \vec{q}_r = \int_{\Omega=0}^{4\pi}\int_{\eta=0}^{+\infty}(\kappa_{\eta,m} I_\eta - \kappa_{\eta,m} I_{\eta b})\,d\eta\, d\Omega \tag{3}$$