

# COMPARISON OF TWO STATISTICAL NARROW BAND MODELS FOR NON-GRAY GAS RADIATION IN PLANAR PLATES

*Huaqiang Chu*<sup>\*</sup>, *Fei Ren*, *Yan Wei*

School of Energy and Environment, Anhui University of Technology, Ma'anshan 243002, PRC

<sup>\*</sup> Huaqiang Chu; E-mail: hqchust@163.com

*Non-gray gas radiation analysis and comparison are conducted by combining a ray tracing method and two statistical narrow band (SNB) spectral models, namely the Goody SNB model and the Malkmus SNB model. In this paper, gas radiation in real gas containing H<sub>2</sub>O, H<sub>2</sub>O/N<sub>2</sub>, or H<sub>2</sub>O/CO<sub>2</sub>/N<sub>2</sub> mixtures at 1 atm in planar plates was studied. Comparisons between these models are performed using the latest narrow-band database. The present computations are validated by reproducing the published results in the literature. The radiative source term, the wall fluxes, the narrow-band radiation intensities along a line-of-sight and the computing time are all compared. From the comparisons, it is found that the Malkmus SNB model is somewhat superior to the Goody SNB model and the former is preferred in engineering application.*

*Key words: polycrystalline silicon, chemical vapor deposition, deposition characteristics*

## 1. Introduction

Radiative transfer plays a key role in high temperature equipment or processes such as boilers, industrial furnaces, and combustors. Accurate analysis of those radiation problems is closely linked with the radiative properties of gases because of the existence of water vapor, carbon dioxide, carbon monoxide or a mixture of these gases in these problems. The radiative properties of these gases exhibit very strong spectral dependence in the near-infrared region at temperatures relevant to combustion. The grey gas assumption, however, is often made in fundamental and applied combustion and flame studies. In many practical applications, it has been well established that the commonly used grey gas model for systems containing combustion gas cannot provide reliable predictions [1, 2]. Thus, we must consider the non-grey radiation properties of real gases.

The complex spectral dependence of the gas radiation makes the determination of spectral radiation properties very difficult. However, significant progress has been made in the development of the spectral models. Nowadays, there are many methods or models to describe the non-grey radiative properties of gases. These approximate methods may be loosely put into four groups as described by Modest [2]: Line by Line (LBL) model, narrow band models, wide band models, and global models.

The radiative heat transfer in absorbing-emitting gas mixtures can be most accurately predicted by the LBL approach, but this model requires large computer resources and computational time and relies on the High Resolution Transmission Molecular Database (HITRAN) [3] and its extension HITEMP [4]. At present, LBL models are used only for benchmark solutions to validate the approximate methods. The SNB model, one of the narrow band models, can lead to results that agree closely with LBL model with good accuracy. Although the last two models (SLW and FSK) still belong to global models, they can produce fairly accurate results provided the reference temperature is carefully selected for the problem at hand [5-10].

In the last ten years, the SNB models have received renewed attention due to the rapid development in computers and interest for accurate analyses of radiation. There are two well known SNB models: the Goody

SNB model and the Malkmus SNB model [11-19]. In order to analyze radiative heat transfer, many numerical methods have been developed to solve RTE, examples being the discrete ordinate method (DOM) and the Monte Carlo Method (MCM). These methods have both advantages and disadvantages, so readers should choose suitable methods according to their problems. Detailed descriptions of these methods are available in the literature, e.g. Modest [1] and Siegal and Howell [20]. The ray-tracing method along with the SNB models was employed by Liu et al. (1998) [16] and Marakis [21]. In the present work, it was used to solve the RTE.

This study concerns non-grey gas radiation in parallel plates using the Goody SNB model and the Malkmus SNB model. Although a similar work was conducted by Marakis [21] using out-of-date narrow-band databases for H<sub>2</sub>O, the present study employed the latest available narrow-band database, Soufiani and Taine [18], and considered mixtures containing H<sub>2</sub>O and CO<sub>2</sub>. In addition, we also compared spectrally resolved radiation intensities from the two SNB models.

## 2. Non-gray gas radiation methods

Narrow band Formulation The spectral RTE for an absorbing, emitting, but non-scattering medium can be written as given by Siegel and Howell [20]

$$\frac{\partial I_v}{\partial s} = -\kappa_{av} I_v + \kappa_{av} I_{bv} \quad (1)$$

The corresponding boundary spectral radiation intensity at a diffuse wall is given as

$$I_v(s_w, \Omega) = \varepsilon_{wv} I_{bwv} + \frac{(1 - \varepsilon_{wv})}{\pi} \int_{\hat{n} \cdot \Omega' > 0} |\hat{n} \cdot \Omega'| I_v(s_w, \Omega') d\Omega' \quad (2)$$

After the spectral radiation intensity is calculated, the total (spectrally integrated) net radiative flux can be obtained from the relation

$$q(x_i) = \sum_{all \Delta v} \left( \sum_{n=1}^N \mu \bar{I}_{v,n,i} w_n \right) \Delta v \quad (3)$$

The radiative source term or the divergence of heat flux,  $-dq/dx$ , of this one-dimensional problem in the medium is then given by

$$-\frac{dq}{dx} = -\frac{q_{i+1} - q_i}{x_{i+1} - x_i} \quad (4)$$

SNB models For an isothermal and homogeneous path-length  $L$  at total pressure  $p$  and molar fraction  $f$ , the narrow band averaged transmittance is given by the Goody SNB model and the Malkmus SNB model (Ludwig et al. [22]) as, respectively,

$$\bar{\tau}_{Gv}(L) = \exp \left[ -SL / \sqrt{1 + \frac{SL}{\pi B}} \right] \quad (5)$$

and

$$\bar{\tau}_{Mv}(L) = \exp \left[ -\frac{\pi B}{2} \left( \sqrt{1 + \frac{4SL}{\pi B}} - 1 \right) \right] \quad (6)$$

where  $L$  is the optical length,  $B = 2\bar{\beta}_v/\pi^2$ ,  $S = \bar{k}_v f p$ , and  $\bar{\beta}_v = 2\pi\bar{\gamma}_v/\bar{\delta}_v$ . The mean narrow band parameters  $\bar{\gamma}_v$ ,  $\bar{\delta}_v$  and  $\bar{k}_v$  for H<sub>2</sub>O and CO<sub>2</sub> have been given by Ludwig et al. [22] and Soufiani et al. [18,23,24], but these databases are out-of-date and may yield inaccurate results. More recently, an updated data set of these parameters has been made available [24] for CO<sub>2</sub>, H<sub>2</sub>O and CO for the much wider temperature range. Further details of this data set can be found in Ref. [18,24].

For a non-isothermal and/or inhomogeneous path, the Curtis-Godson approximation [26] is commonly used to obtain equivalent band parameters. Equivalent band parameters  $\bar{k}_v$  and  $\bar{\beta}_v$  are given by averaging  $k$  and  $\beta$  over the optical path  $U$  of the column as

$$U = \int_0^l p x ds \quad (10)$$

$$\bar{k}_{eq} = \frac{1}{U} \int_0^l p x k ds \quad (11)$$

$$\bar{\beta}_{eq} = \frac{1}{U} \int_0^l p x k \beta ds \quad (12)$$

Following Kim et al. [14], the overlapping band is treated as a new band.

### 3. Results and discussion

In order to compare the two SNB models, four different cases for the concentration and temperature distributions between two infinite planar plates are tested. Three problems for H<sub>2</sub>O/N<sub>2</sub> mixture were first employed by Kim et al. [14] and the last one was calculated by Liu et al. (2000) [25] using the SNB-CK model for a H<sub>2</sub>O/CO<sub>2</sub>/N<sub>2</sub> mixture. In the four cases, the wall surfaces were assumed to be black and the medium was at a uniform total pressure of 1 atm. The same spatial and angular discretizations have been adopted for all the test cases. The planar geometry was subdivided into 20 sublayers and the polar angle into 20 intervals. The physical explanation for the four cases were given in Kim et al. [14], Liu et al. (1998) [16], and Liu et al. (2000) [25]. Reference results for the problems presented are those given in Kim et al. [14], Liu et al. (1998) [16], and Liu et al. (2000) [25].

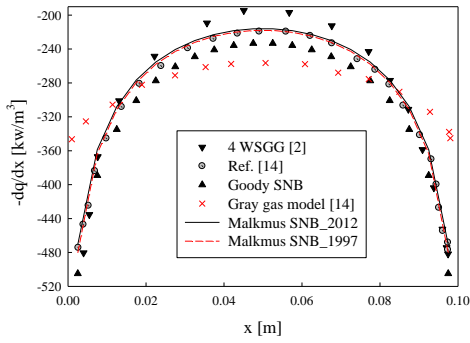
#### 3.1. Assessment of the radiative source term

*Isothermal homogeneous medium (Case 1)* In the first case, the two walls were held at 0 K. The medium between the two planar plates is filled with 100 percent water vapor at a uniform temperature of 1000 K. Two wall separation distances, of 0.1 m and 1 m, were used.

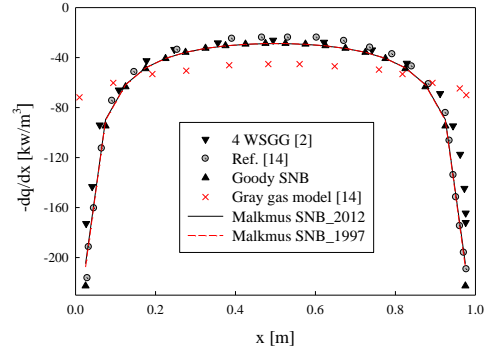
Figures 1 and 2 show the predicted radiative source distributions using the Goody and the Malkmus SNB models for the two different separation distances. The discrepancies between the results obtained from the two SNB models are found to be large for the smaller separation distance of 0.1 m; while the predictions are in better agreement with each other for the larger separation distance of 1 m. In these figures, the WSGG model was that developed by Song [2] based on the EWB model (Edwards and Balakrishnan [5]), while the SNB model and the grey gas model were adopted by Kim et al. [14]. The WSGG model also gives reasonable results, whereas the results of the gray gas model are far off from the reference solution (Kim et al. [14]). Note that the results of the Malkmus SNB model are in excellent agreement with those of the reference solution for both optical lengths. The magnitude of the heat source becomes smaller as the optical thickness of the medium increases.

*Isothermal inhomogeneous medium (Case 2)* For this case, the gas is maintained at a uniform temperature of 1000 K, but the medium is a non-uniform mixture of H<sub>2</sub>O/N<sub>2</sub> with a parabolic H<sub>2</sub>O concentration profile given by  $f_{H_2O} = 4(1 - x/L)x/L$  the separation distance is 1 m.

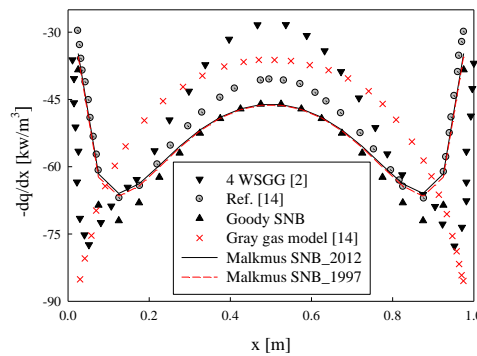
Figure 3 presents the results of the source term from different gas models. The Goody SNB model result does not show significant difference from that of the Malkmus SNB model in the middle of the medium or close to the walls. However, there are relatively large differences around the two minima. The W-shaped profile of the source term is well captured by the two SNB models. The predictions of the WSGG model and the gray gas model are much worse than those of the two SNB models, especially for the gray gas model which even fails to capture the W-shaped distribution.



**Figure 1. Distributions of the radiative source term for the homogeneous and isothermal case with the separation distance of 0.1 m (Case 1).**

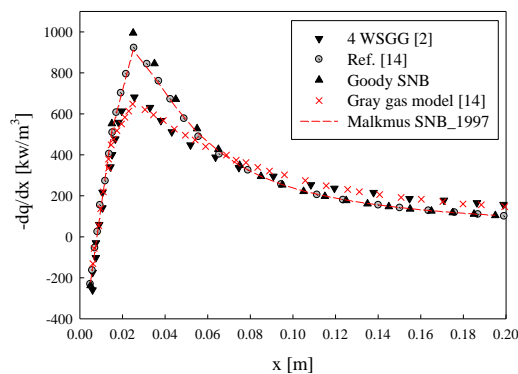


**Figure 2. Distributions of the radiative source term for the homogeneous and isothermal case with the separation distance of 1 m (Case 1).**



**Figure 3. Distributions of the radiative source terms for the isothermal case with parabolic water vapor concentration profile (Case 2).**

*Non-isothermal homogeneous medium (Case 3)* The third problem analyzed has a boundary layer type temperature profile. The medium is again pure water vapor, the left plate is at 1500 K and the right plate is at 300 K. The distance between the plates is 0.2 m. The calculated source term distributions are compared in Fig. 4. From Figure 4, a similar observation to that in Case 1 can be made. Both SNB models predict the sharp rise of the radiative source term near the left wall with the results of the Malkmus model in better agreement with the reference solution. However, the WSGG model and the gray gas model cannot resolve the rapid change in the source term distribution.



**Figure 4. Distributions of the radiative source term for the boundary-layer type temperature case with pure water vapor (Case 3).**

### 3.2. Comparison of the net wall heat fluxes and computing time

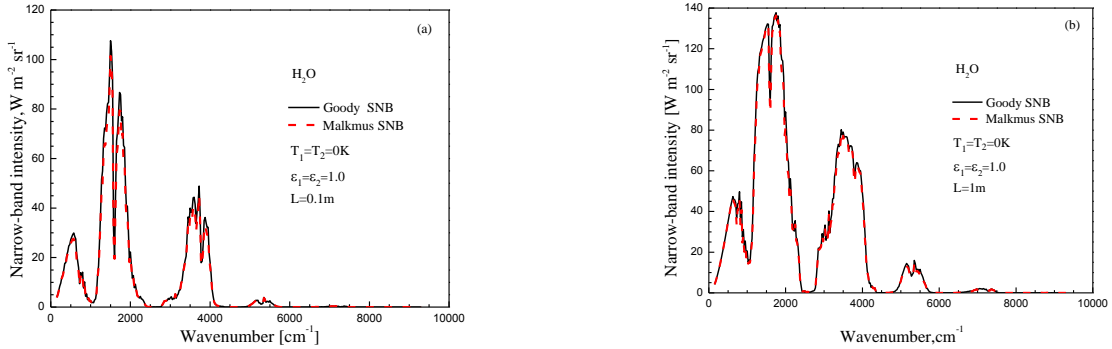
The net heat fluxes at the boundary and computing time for all the cases are summarized in Table 1. The discrepancy between the two SNB models is evident, although it is quite small, from the table.

**Table 1. Net wall heat fluxes (kW/m<sup>2</sup>) and computing time (s) for the four cases**

Cases	Length (m)	Kim et al. [14]		Malkmus SNB		Goody SNB	
		Heat flux (kW/m <sup>2</sup> )	Time (s)	Heat flux (kW/m <sup>2</sup> )	Time (s)	Heat flux (kW/m <sup>2</sup> )	Time (s)
Case 1	0.1	-14.3	/	-14.2	3.14	-15.1	3.25
	1.0	-28.2	/	-30.3	3.20	-31.3	3.34
Case 2	1.0	-25.2	/	-27.0	3.20	-28.1	3.34
Case 3	0.2	277.4	/	271.7	3.16	271.2	3.25

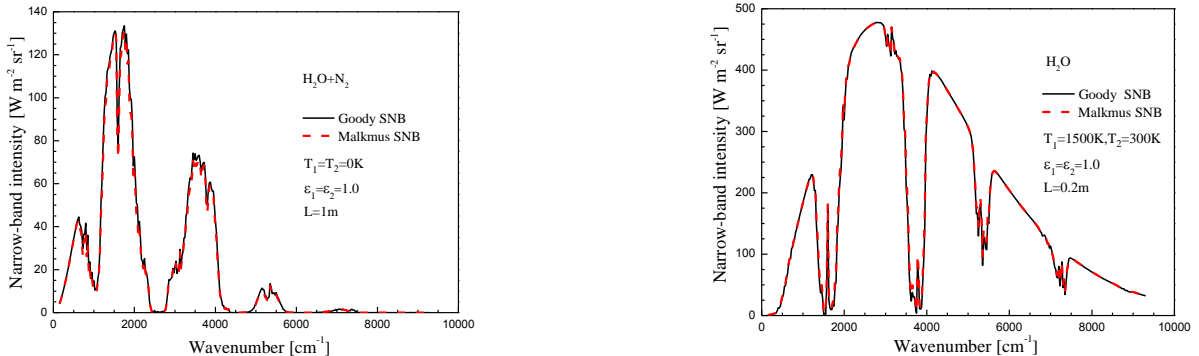
### 3.3. Narrow band intensities along a line-of-sight

Figures 5, 6 and 7 compare narrow band intensities along a line-of-sight (at  $x = L$  and along the positive  $x$  direction) for the four cases mentioned above. From these figures, we can see that there are not significant differences in the narrow band intensities obtained using the Goody SNB model and Malkmus SNB model; however, results of the former are in general slightly higher than those of the latter. This is consistent with the somewhat higher radiative source term and heat flux from the Goody SNB model shown earlier. Figure 5 shows that the narrow band intensities with a greater optical length vary more than those with a shorter length. It is found that variations of the narrow band intensities also become significant when the medium of pure water is replaced by a mixture of H<sub>2</sub>O, CO<sub>2</sub> and N<sub>2</sub> as shown in Figure 7. The treatments for the overlapping bands (such as 450 to 1200, 1950 to 2450 and 3300 to 3800) of H<sub>2</sub>O and CO<sub>2</sub> have been discussed by Liu et al. (2001) [27]. In the present paper, we employed the same treatment as that of Kim et al. [14]. In future work, we will investigate the treatment of the overlapping bands to improve the accuracy of the model.



**Figure 5. Comparisons of narrow-band intensities for case 1 with two optical paths (a) 0.1 m and (b) 1**

**m.**



**Figure. 6. Comparisons of narrow-band intensities for Case 2.**

**Figure.7. Comparisons of narrow-band intensities for case 3**

#### 4. Conclusions

Four test problems have been investigated to compare the Goody SNB model and the Malkmus SNB model using the recently available narrow-band database in the literature. The radiative source term, the wall fluxes, the narrow band intensities along a line-of-sight and the computing time were investigated. In general the differences between the two SNB models are fairly small. The following observations were made from the results of the present study:

- (1) For the isothermal homogeneous medium, Case 1, results of the Malkmus model exhibit relatively large differences from those of the Goody model when the optical length is small. However, the differences become smaller with the increase of the optical length.
- (2) For the isothermal inhomogeneous medium, Case 2, results of the two SNB models depart from the literature solution, with those of the Malkmus model in better agreement with the benchmark solution.
- (3) For the non-isothermal cases, Cases 3, the Malkmus SNB model is again more accurate than the Goody model, judged by the closer agreement between the results of the Malkmus model and solutions from the literature.
- (4) For the CPU time required for the four problems, the Malkmus model is slightly more efficient than the Goody model.
- (5) The differences in the narrow-band radiation intensities from both SNB models are fairly small for the four cases considered.

More recently, the DRESOR method based on the MCM for RTE has been proposed by Zhou et al. [28, 29] for gray media. By this method, the intensity with high directional resolution at any point can be obtained with high precision. This method will be extended for non-gray gas radiation in the near future.

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#### Nomenclature

$f$	Species molar fraction	$x$	Cartesian coordinates $m$
$I$	Radiation intensity $W / m^2 sr$	<b>Greek symbols</b>	
$I_\nu$	Spectral radiation intensity	$\bar{\beta}_\nu$	Mean line-width to spacing ratio
	$W / m^2 \cdot sr \cdot cm^{-1}$	$\bar{\gamma}_\nu$	Mean half-width of an absorption line
$k_\nu$	Mean line-intensity to spacing ratio		$cm^{-1}$
	$cm^{-1} \cdot atm^{-1}$	$\bar{\delta}_\nu$	equivalent line spacing $cm^{-1}$
$\bar{k}_\nu$	Equivalent mean line-intensity to spacing ratio $cm^{-1} \cdot atm^{-1}$	$\Delta\nu$	Wavenumber interval $cm^{-1}$
$L$	Separation distance between parallel walls $m$	$\nu$	Wavenumber $cm^{-1}$
$p$	Pressure $atm$	$\mu$	Direction cosines
$q$	Heat flux density $kW / m^2$	$\tau_\nu$	Spectral transmittance
$s, s'$	Position variables $m$		

## Subscripts

$n$	Angular discretization index
$w$	Wall
$b$	Blackbody
$i$	Spatial discretization (along a line of sight) index

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