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Calculations of gas thermal radiation transfer in one-dimensional planar enclosure using LBL and SNB models

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ABSTRACT

Thermal radiation transfer in one-dimensional enclosure between two parallel plates filled with real gases, namely CO₂, H₂O, or their mixtures, was calculated using the line-by-line approach and the statistical narrow-band model. Line-by-line calculations were carried out using the HITEMP1995, HITRAN2004, HITRAN2008, HITEMP2010, and updated CDSD-1000 databases. This study demonstrates the importance of spectral database to the accuracy of line-by-line calculations through a systematic comparison of line-by-line results using different databases. Calculations of the statistical narrow-band model were conducted using the EM2C narrow-band database. The strong dependence of line-by-line results on the spectral database was demonstrated through several gas radiation transfer problems in planar-plate enclosure containing real gases of both isothermal or non-isothermal and uniform or non-uniform concentrations at 1 atm. Fairly significant differences were found between the line-by-line results using the HITEMP2010 database and those using older databases. Very good agreement in both the wall heat flux and the radiative source term was observed between the line-by-line results using the HITEMP2010 database and the results of the statistical narrow-band model in all the cases tested, confirming the EM2C narrow-band parameters for both H₂O and CO₂ are accurate. For cases involving CO₂ the line-by-line results using the HITEMP2010 database are in excellent agreement with those using the updated CDSD-1000 databases. The line-by-line results based on the HITEMP2010 database should be used as benchmark solutions to evaluate the accuracy of other approximate models.

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1. Introduction

Radiative properties of CO₂ and H₂O have received continuous research attention in the last few decades mainly because they are required to model radiative transfer in various applications, such as remote-sensing, atmosphere science, heat transfer, and combustion and fires. The last two decades have witnessed a rapid development of efficient and yet accurate non-gray gas radiative property models for the ultimate application to large-scale three-dimensional engineering problems. Accurate CFD modeling of the recently developed oxy-fuel combustion technologies has generated renewed interest in assessing the suitability of traditional weighted-sum-of-gray-gases (WSGG) models and developing efficient and accurate gas radiative property models under very high concentrations of CO₂ for large-scale and 3D CFD calculations [1,2].

The extremely rapid variation of the radiative properties of real gases (primarily CO₂ and H₂O in combustion) with wavelength makes it difficult to predict thermal radiation transfer accurately

and efficiently. Various models have been developed in the literature over the last few decades, which include the line-by-line (LBL) model, narrow band models, wide band models, and global models. Comprehensive reviews of these models can be found in [3–6].

The statistical narrow band (SNB) model [7,8] is the most successful narrow-band model that can lead to results in close agreement with those from the LBL model. Based on the blackbody-weighted transmission function and the blackbody-weighted cumulated distribution function, André and Vaillon [9] developed the spectral-line moment-based (SLMB) model, which can be regarded as further development of the SNB model. To gain better computational efficiency for thermal radiation transfer calculations, Edwards and Balakrishnan [10] developed the exponential wide-band (EWB) model, which is the most successful wide-band model. The above band models (SNB, EWB) provide transmissivity, rather than the fundamental gas absorption coefficient required in the differential form of the radiative transfer equation (RTE). Consequently, these band models are compatible only with the RTE in integral form but cannot be readily coupled with the RTE in differential form. The implication is that these band models cannot be coupled with various techniques developed to solve the differential form RTE, such as the discrete ordinates method (DOM) [11], the

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Nomenclature

c	speed of light in vacuum (m s^{-1})
E''	the lower state energy of the transition (cm^{-1})
f	species molar fraction
F	Lorentz profile (cm)
h	Planck constant (J s)
I	total radiation intensity ($\text{W m}^{-2} \text{sr}^{-1}$)
I_v	spectral radiation intensity ($\text{W m}^{-2} \text{sr}^{-1} \text{cm}^{-1}$)
k_B	Boltzmann constant (J K^{-1})
$\bar{k}_v$	equivalent mean line-intensity to spacing ratio ($\text{cm}^{-1} \text{atm}^{-1}$)
L	separation distance between parallel walls (m)
N	molecule number density ($\text{mol (m cm}^{-2})^{-1}$)
P	pressure (atm)
q	heat flux density (kW m^{-2})
Q_r	rotational partition functions of the absorbing gas
Q_v	vibrational partition functions of the absorbing gas
s, s'	position variables (m)
S	line intensity ($\text{cm}^{-1} (\text{mol cm}^{-2})^{-1}$)
T	temperature (K)
x	Cartesian coordinates (m)

Greek symbols

$\bar{\beta}_v$	mean line-width to spacing ratio
κ_v	spectral absorption coefficients (m^{-1})
γ	line half-width at half-maximum (HWHM) (cm^{-1})
γ_{air}	air-broadened half-width at 296 K ($\text{cm}^{-1} \text{atm}^{-1}$)
γ_{self}	self-broadened half-width at 296 K ($\text{cm}^{-1} \text{atm}^{-1}$)
$\bar{\gamma}_v$	mean half-width of an absorption line (cm^{-1})
δ_v	equivalent line spacing (cm^{-1})
Δv	wavenumber interval (cm^{-1})
ν	wavenumber (cm^{-1})
τ_v	spectral transmittance
Ω	direction of propagation or solid angle (sr)

Subscripts

b	blackbody
i	spatial discretisation (along a line of sight) index
n	angular discretisation index
w	wall

Monte Carlo Method (MCM) [12,13], the zone method (ZM) [14], or the DRESOR method [15]. Although the band models can be readily coupled with solution methods developed to solve the integral form RTE, such as the ray-tracing method and the discrete transfer method, the problem is that these solution methods are in general more computationally demanding than those for the differential form of the RTE and are difficult to account for scattering. These drawbacks of the band models can be overcome by employing the band models through the cumulative absorption coefficient distribution function methodology, which leads to the availability of absorption coefficients [16–20]. The WSGG model, originally introduced by Hottel and Sarofim [21], is a representative of the global non-gray models, being more sophisticated and somewhat more accurate than the gray gas model. The WSGG model gained popularity in engineering applications due to its efficiency and improved accuracy over the gray gas model, especially after the work of Modest [22] who showed that this model could be used with any RTE solver. As shown in Ref. [23], the WSGG model yields poor accuracy but a low computation time compared to the SNB model. Based on the absorption-line blackbody distribution function, Denison [24] and Solovjov and Webb [25,26] developed and extended the spectral line-based weighted-sum-of-gray-gases (SLW) to overcome the shortcomings and to improve the accuracy of the conventional WSGG model. Recently, Modest and co-workers [27,28] developed the full-spectrum correlated-k (FSCK) and multi-scale full-spectrum correlated-k (MSFSCK) methods. In essence, the SLW and FSCK models are similar to the absorption distribution function (ADF) and the absorption distribution function fictitious gas (ADFFG) models [29,30], which use the full-spectrum absorption coefficient distributions calculated from high-resolution databases. Although the SLW and FSCK still belong to global models, they possess two important advantages over the band models. First, they are much more computationally efficient and can be very accurate when about 10–20 gray gases (or equivalently quadrature points) are used and provided the reference temperature is carefully selected for the problem at hand. Secondly, they can be coupled with any RTE solvers and account for gray scattering with ease. These models have not gained widespread use in CFD modeling of large-scale combustion problems, mainly because it is still somewhat too expensive to incorporate these models into the flow and temperature field calculations in a fully coupled fashion.

The LBL approach, the most accurate spectral model of all, requires calculation of gases radiative properties at a spectral resolution comparable to individual line width (on the order of 0.01 cm^{-1}) characterized by half-width at half maximum (HWHM). At such resolution the whole spectrum relevant to radiative heat transfer consists of millions of single lines, i.e., the RTE has to be solved millions of times. Hence, the LBL approach is very computationally demanding. LBL calculations have become an attractive method for radiative transfer with the further development of computing capacity [31]. However, it is unlikely that they can be applied to practical multidimensional engineering applications in the foreseeable future. On the other hand, the LBL approach is very valuable to develop benchmark solutions for evaluating the accuracy of other approximate models. Although the LBL approach is supposed to provide very high accuracy results for radiation heat transfer problems, it is expected that its results are dependent on the quality/accuracy of the spectral database used in such calculations, since LBL calculations rely on a high-resolution gas property database that resolves individual spectral lines. Earlier versions of high resolution spectral databases, such as HITRAN [32–34] and HITEMP [35], suffer from the limitation that they are applicable only for low to medium temperatures (up to about 1000 K) due to absence of the so-called hot lines. The updated HITEMP database, HITEMP2010 [36], includes a lot more spectral lines and can be applied to radiative transfer calculations at temperatures relevant to combustion problems (up to 3000 K). As indicated earlier, the newly developed accurate and efficient global models, i.e., SLW, FSCK, and SLMB, share a common starting feature: their fundamental model parameters are obtained from a high-resolution spectral LBL database. Unfortunately, there is no accurate spectroscopic data available at high temperatures, though various efforts have been made. Up to date, HITEMP2010 is the most accurate database for H_2O and CO_2 , at high temperatures. Prior to the availability of HITEMP2010, earlier versions of LBL databases, such as HITEMP1995, HITRAN2004, and HITRAN2008, had been employed for LBL calculations. The CDSD database [37–40], which is more accurate for CO_2 , also was included in the present evaluation study.

In this work, LBL programs were developed to calculate the absorption coefficients of CO_2 and H_2O and radiative heat transfer in one-dimensional parallel-plate enclosures containing mixtures

of $\text{H}_2\text{O}/\text{N}_2$, CO_2/N_2 , or $\text{CO}_2/\text{H}_2\text{O}/\text{N}_2$. The RTE in differential form was solved using DOM. Calculations were carried out in several cases of various distributions of radiating gas concentrations (homogeneous or inhomogeneous) and temperature (isothermal or non-isothermal) and different distances between the plates. Results of the SNB model have often been used as benchmark solution in the absence of LBL results in the literature. It is therefore of interest to evaluate the SNB results against the LBL ones. For this purpose, SNB model calculations using a ray-tracing solver were also conducted.

The objectives of this study are threefold: (1) to evaluate the effect of spectral database on the LBL results of radiative heat transfer by performing LBL calculations using several different spectral databases, including HITEMP1995, HITRAN2004, HITRAN2008, HITEMP2010, and CDSD-1000 (updated), (2) to evaluate the accuracy of the SNB model by comparing the SNB results obtained using the EM2C SNB parameters against the LBL results using the HITEMP2010 database, and (3) to provide updated benchmark solutions of radiative heat transfer with the assumption that HITEMP2010 is currently the most accurate spectral database at high temperatures. In the next section, the LBL method, several high-resolution spectral databases, and the SNB model are first presented. The numerical results are then presented and discussed. Finally some conclusions are drawn based on the present results.

2. Models

2.1. The line-by-line (LBL) method

In the LBL approach, the spectral absorption coefficient at a wavenumber ν , κ_ν , contributed by all individual lines is given as [32,41,42]

$$\kappa_\nu = N \sum_i S_i(T) F_i(\nu) \quad (1)$$

where N is the molecule number density of the radiating species under consideration; S_i is the line intensity of the i th line, $F(\nu)$ is the line shape profile [32],

In applications where collision broadening is dominant, such as in radiative heat transfer, a spectral line follows the Lorentz profile expressed as

$$F_i(\nu) = \frac{\gamma_i}{\pi[(\nu - \nu_i)^2 + \gamma_i^2]} \quad (2)$$

where γ is the half-width at half-maximum (HWHM) of the line. The line half-width can be calculated using the following relation given in [32]

$$\gamma = \left(\frac{T_0}{T}\right)^n [\gamma_{\text{air}}(P - P_s) + \gamma_{\text{self}} P_s] \quad (3)$$

where $T_0 = 296$ K (for the CDSD-1000 database $T_0 = 1000$ K) is the reference temperature, T , n , P , P_s , γ_{air} , γ_{self} are the gas temperature, the coefficient of temperature dependence, the total pressure, the gas partial pressure, the air-broadened half-width, and the self-broadened half-width, respectively. The line intensity $S_i(T)$ is obtained from the following expression, given in [32]

$$S_\nu(T) = S_\nu(T_0) \frac{Q_{\nu 0} Q_{r 0}}{Q_\nu(T) Q_r(T)} \exp \left[\frac{hcE''}{k_B} \left(\frac{1}{T_0} - \frac{1}{T} \right) \right] \frac{1 - \exp(-hc\nu/k_B T)}{1 - \exp(-hc\nu/k_B T_0)} \quad (4)$$

where Q_ν , Q_r are vibrational and rotational partition functions of the absorbing gas, respectively. E'' is the lower state energy of the transition, ν is the associated transition wavenumber between the initial and final energy state, h is the Planck constant, c is the speed of light in vacuum, k_B is the Boltzmann constant. The line parameters for

H_2O and CO_2 , such as line intensities $S_i(T_0)$, energy E'' , and the spectral position of the line ν_i , under atmospheric conditions at the reference temperature can be obtained from a high resolution spectral database. For a gas mixture containing more than one radiating species, the spectral absorption coefficient of the mixture is simply the summation of contribution from all the radiating species.

In this study, a uniform spectral resolution of 0.02 cm^{-1} (i.e., $\Delta\nu = 0.02 \text{ cm}^{-1}$) was chosen for wavenumbers between 150 and 9300 cm^{-1} to conduct LBL calculations. Higher and lower spectral resolutions were also considered in the numerical experiments. It was found that use of higher resolutions than $\Delta\nu = 0.02 \text{ cm}^{-1}$ had negligible influence on the results but significantly increased the computing time. On the other hand, use of lower resolutions led to results that considerably deviate from those obtained at higher resolutions. Therefore, the spectral resolution of $\Delta\nu = 0.02 \text{ cm}^{-1}$ was found optimal between accuracy and efficiency. Furthermore, a spectral distance of 20 HWHM between the spectral line center and the wavenumber under consideration was used as the cut-off distance, i.e., if the spectral distance between the center of a spectral line and the spectral location of interest is greater than 20 HWHM the contribution of this spectral line to the absorption coefficient at the wavenumber under consideration is neglected. Numerical experiments were also carried out for other cut-off spectral distances and a 20 HWHM was again found to be optimal between accuracy and efficiency.

Once the spectral absorption coefficients over the whole spectrum at a spectral resolution of $\Delta\nu = 0.02 \text{ cm}^{-1}$ are calculated from the LBL method described above for given species concentration and temperature distributions, the spectral radiation intensity, the total net radiative flux, and the radiative source term can be obtained by solving the RTE.

In an emitting-absorbing medium, the RTE and its corresponding boundary condition for the spectral radiation intensity at a diffuse wall can be written as follows [5,6]:

$$\frac{\partial I_\nu(s, \Omega)}{\partial s} = -\kappa_\nu(s) I_\nu(s, \Omega) + \kappa_\nu(s) I_{b\nu}(s), \quad (5)$$

$$I_\nu(s_w, \Omega) = \varepsilon_{w\nu} I_{b\nu\nu} + \frac{(1 - \varepsilon_{w\nu})}{\pi} \int_{\hat{n} \cdot \Omega' < 0} |n \cdot \Omega'| I_\nu(s_w, \Omega') d\Omega', \quad (6)$$

for $n \cdot \Omega' > 0$

where $I_{b\nu}(s)$ and $I_{b\nu\nu}$ are the blackbody radiative intensity inside the medium and at the wall, respectively, and $\varepsilon_{w\nu}$ is the wall spectral emissivity.

For radiative heat transfer in one-dimensional parallel-plate enclosures containing absorbing-emitting gas, the RTE can be solved accurately using DOM in one-dimensional Cartesian coordinates. In this study, the DOM formulation presented by Liu et al. [43] was followed. The spectral radiation intensity at a nodal point p along a discrete direction m with a positive direction cosine ξ^m can be written as [43]

$$I_{\nu,p}^m = \frac{(\xi^m / \omega_x^m) I_{\nu,w}^m + \kappa_\nu I_{b\nu,p} \Delta x}{\xi^m / \omega_x^m + \kappa_\nu \Delta x} \quad (7)$$

where $I_{\nu,w}^m$ is the upstream spectral radiation intensity along the discrete direction m , ω_x^m is the weighting factor to relate the radiation intensity at the nodal point to the upstream ($I_{\nu,w}^m$ for positive ξ^m) and downstream ($I_{\nu,e}^m$ for positive ξ^m) values, i.e.,

$$I_{\nu,p}^m = \omega_x^m I_{\nu,e}^m + (1 - \omega_x^m) I_{\nu,w}^m \quad (8)$$

The positive scheme described by Liu et al. [43] was employed where the weighting factor is calculated as

$$\omega_x^m = \max(0.5, \omega_x^{m'}) \quad (9)$$

where $\omega_x^{m'} = 1 - \alpha/\kappa_v$ and $\alpha = \zeta^m/\Delta x$. Eq. (7) is solved for each wavenumber. A similar expression to Eq. (7) can be obtained for radiation intensities along directions with negative direction cosines.

Once the intensity field is obtained, the net radiative flux and the source term can be calculated as

$$q(x_i) = \sum_{\text{all } \Delta v} \left(\sum_{m=1}^M \zeta^m I_{v,i}^m W^m \right) \Delta v \quad (10)$$

and

$$\left(-\frac{dq}{dx} \right)_p = -\frac{q_{i+1} - q_i}{x_{i+1} - x_i} \quad (11)$$

It is noted that the net radiative flux is evaluated at the cell boundaries, while the radiative source term is evaluated at nodal points (cell center).

2.2. Databases

To investigate the effect of high-resolution spectral database on the results of LBL method for radiative heat transfer, five databases, i.e., HITEMP1995, HITRAN2004, HITRAN2008, HITEMP2010, and CDSD-1000 (only for CO₂), were employed to conduct LBL calculations, since HITRAN and HITEMP databases are the most complete and popular databases. These databases all provide the information of the relevant parameters for all spectral lines of different absorbing/emitting gases, including line intensities, positions (wavenumber), half-widths, lower level energy, etc. under the standard conditions (296 K for HITRAN and HITEMP, or 1000 K for CDSD, and 1 atm). Table 1 lists the number of spectral lines in different versions of HITRAN and HITEMP databases considered for CO₂ and H₂O, and CDSD-1000 (for CO₂ only) over the entire spectrum and the spectral region of interest to the present study.

The HITRAN database for absorbing/emitting gases at atmospheric temperature was first developed nearly three decades ago and has been continuously updated over the years (1973, 1986, 1992, 1996, 2000, 2004, 2008). The latest edition contains line-by-line parameters for 42 molecules. Although primarily intended for atmospheric studies, important combustion species, such as CO₂, H₂O, NO, NO₂, OH, CH₄ and C₂H₂, are also included. However, it should be pointed out that the HITRAN database is created only for low temperature conditions. The HITRAN database covers the line transitions accurately at temperature range below 1000 K. Above this temperature, there are many hot lines to appear with the increase in temperature that are missing in HITRAN databases. HITEMP was developed for high temperature conditions. The HITEMP2010 database includes a lot more hot lines that are

absent in HITRAN. Therefore, the HITEMP2010 database should be significantly more accurate at high temperatures relevant to combustion. The current database contains five molecules H₂O, CO₂, CO, NO, and OH relevant to combustion. The HITRAN and HITEMP databases were discussed in detail in the literature [44,45]. Based on these databases, CDSD (only for CO₂) was developed by Tashkun et al. [37–40]. CDSD-1000 (updated) [40] is an updated version and is used in this study. It is worth noting that a hybrid database, in which the line properties of H₂O were taken from HITEMP2010 while the line properties of CO₂ were from CDSD-1000 (hereafter HITEMP2010 + CDSD-1000), is also used in the present study.

2.3. The statistical narrow band (SNB) model

For an isothermal and homogeneous path-length L containing a radiating gas at a mole fraction f and total pressure p , the SNB model provides the narrow band averaged transmissivity given as [46]

$$\bar{\tau}_v(L) = \exp \left[-\frac{\pi B}{2} \left(\sqrt{1 + \frac{4SL}{\pi B}} - 1 \right) \right] \quad (12)$$

where L is the path 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 H₂O and CO₂ have been reported by Soufiani and Taine [47] as an updated SNB model dataset based on a high resolution spectral database developed at EM2C. This narrow-band dataset covers a wider temperature range from 300 to 2900 K for a uniform bandwidth of 25 cm⁻¹ between 150 and 9300 cm⁻¹. H₂O absorbs and emits radiation at all of the 367 narrow-bands while CO₂ has 96 radiating bands in the following four spectral regions: 450–1200 cm⁻¹ (31 bands), 1950–2450 cm⁻¹ (21 bands), 3300–3800 cm⁻¹ (21 bands), and 4700–5250 cm⁻¹ (23 bands). Further details of this dataset can be found in Soufiani and Taine [47]. It is worth noting that hot lines were included in the high resolution spectral database of EM2C, which was based on HITRAN1992 [48]. The hot lines in the EM2C high resolution spectral database were generated using approximate theoretical and empirical formulas. The updated SNB parameters of CO₂, H₂O, and CO were generated from the EM2C high resolution spectral database.

The SNB model was incorporated into the RTE in integral form. The ray-tracing method described in Refs. [49,50] was used to solve the integral RTE. For a non-isothermal and/or inhomogeneous path, the Curtis–Godson approximation [51] was employed. The overlapping band of gas mixture is treated in a manner as adopted by Kim et al. [52], i.e., using the multiplication property of transmissivity.

3. Results and discussion

The LBL and SNB models were used to calculate radiative heat transfer in six different cases in one-dimensional isothermal/non-isothermal, homogeneous/inhomogeneous gases between two planar plates containing H₂O/N₂, CO₂/N₂, or CO₂/H₂O/N₂ mixtures. Numerical calculations were conducted using 20 uniform control volumes and the T₃ angular quadrature set with 72 directions in the entire 4 π solid angle. Further refinement in either the spatial or angular refinement has negligible influence on the results, in agreement with the findings of Liu et al. [49] with regard to the effect of grid size.

Some test cases were considered previously by several researchers using different models. For all the cases, the wall surfaces were assumed to be black and the medium was at a uniform total pressure of 1 atm. For the last two cases, we considered two scenarios relevant to air combustion (Case 5), where the CO₂ concentrations are fairly low, and oxy-fuel combustion with flue gas

Table 1
Number of spectral lines and the spectral coverage range in HITRAN and HITEMP databases for CO₂ and H₂O and in the updated CDSD-1000 database for CO₂.

Database	H ₂ O	Spectral coverage (cm ⁻¹)	CO ₂	Spectral coverage (cm ⁻¹)
HITEMP2010	114,241,164 104,508,960	0–30,000 150–9300	11,193,608 11,159,843	5–12,785 150–9300
HITRAN2008	69,201 43,433	0–25,232 150–9300	314,919 310,948	0–12,784 352–9300
HITRAN2004	63,196 43,435	0–25,232 150–9300	62,913 61,924	0–12,784 442–8309
HITEMP1995	1,283,468 1,033,344	0–24,990 150–9300	1,032,269 1,032,102	157–9648 157–8309
CDSD-1000	– –	– –	360,252 358,969	263–9648 263–9300

Fig. 1. Temperature and CO_2 and H_2O mole fraction distributions for air combustion and oxy-fuel combustion scenarios.

Table 2
Descriptions of the six test cases.

Case	Medium	L (m)	T (K)	$f_{\text{H}_2\text{O}}$	f_{CO_2}
1	H_2O	0.1	1000	1.0	–
2	H_2O	1.0	1000	1.0	–
3	CO_2	0.1	2000	–	0.5
4	CO_2	0.5	1500	–	0.1
5	H_2O	1.0	1000	$4(1 - x/L)x$	–
6	$\text{H}_2\text{O} + \text{CO}_2$	0.2	Ref. [52]	1.0	–
7	$\text{H}_2\text{O} + \text{CO}_2$	0.5	See Fig. 1	See Fig. 1	See Fig. 1
8	$\text{H}_2\text{O} + \text{CO}_2$	0.5	See Fig. 1	See Fig. 1	See Fig. 1

recirculation (with the removal of H_2O from the flue gas) (Case 6), where the concentrations of CO_2 are much higher than those in air combustion. The distributions of CO_2 and H_2O mole fraction and temperature are displayed in Fig. 1 under both air combustion and oxy-fuel combustion scenarios. The distributions of CO_2 and H_2O mole fraction and temperature in the air combustion scenario were given in detail by Liu et al. [49]. Under the scenario of oxy-fuel combustion with flue gas recirculation, the CO_2 mole fraction is increased everywhere by 0.6 relative to the distribution under air combustion scenario, while the distributions of H_2O mole fraction and temperature are unchanged. The distributions of temperature and mole fractions of CO_2 and H_2O for the six test cases are summarized in Table 2.

All the calculations were carried out on a Dell Precision T7500 Workstation equipped with dual quad core Intel Xeon 2.93 GHz processors and 12 GB RAM. To illustrate how CPU time demanding LBL calculations can be and how drastic the difference in computational efficiency between the LBL method and the SNB model is, it suffices to mention that the LBL calculations using HITEMP2010 + CDSD-1000 for Case 6, which is the most time consuming case in this study, consumed about 160 h CPU time, while the SNB calculations required only few seconds.

3.1. Isothermal and homogeneous H_2O (Case 1)

In this case, two separation distances between the parallel plates were considered, i.e., $L = 0.1$ m and 1.0 m. Figs. 2 and 3 compare the distributions of the radiative source term and the net radiative flux calculated using the LBL method and the SNB model for the two separation distances, respectively. Also plotted in Figs. 2(a) and 3(a) are the LBL results of Denison [24]. Similar to the EM2C

Fig. 2. Distributions of the predicted local radiative source (a) and net radiative flux (b) for Case 1: uniform temperature of $T = 1000$ K, $f_{\text{H}_2\text{O}} = 1.0$ and $L = 0.1$ m.

high resolution spectral database mentioned earlier, the high resolution spectral database used in the LBL calculations of Denison [24] was also developed based on HITRAN1992 with estimated “hot lines” included from theoretical considerations. The first observation from Figs. 2 and 3 is that the LBL results are sensitive to the spectral database used, especially for the smaller separation distance, Fig. 2. It can be seen from Figs. 2(a) and 3(a) that the LBL model overpredicts the radiative source term when the HITEMP1995 spectral database is used, especially for the smaller separation distance of $L = 0.1$ m between the plates, Fig. 2(a). Similar to the observation of the radiative source term distributions, the LBL results of net radiative heat flux obtained using HITEMP1995 also exhibit the largest deviation from LBL results obtained using the other three more recent databases, Figs. 2(b) and 3(b), especially for the smaller separation distance of 0.1 m, Fig. 2(b). The LBL results shown in Figs. 2 and 3 suggest that the HITEMP1995 spectral database gives rise to large errors, even at an intermediate temperature of 1000 K, and should not be used for LBL calculations of radiative transfer problems. Therefore, it will not be used further in LBL calculations of other test cases.

It can also be seen from Figs. 2 and 3 that the LBL results obtained by HITRAN2004 and HITRAN2008 are very close to each other, especially for the larger separation distance of $L = 1.0$ m, Fig. 3. Overall, the differences between the LBL results from HITEMP2010 and those from HITRAN2004 and HITRAN2008 are relatively small, especially for the larger separation distance, Fig. 3. It is evident from the results shown in Figs. 2 and 3 that there is a clear trend in the LBL results obtained from the oldest database

Fig. 3. Distributions of the predicted local radiative source (a) and net radiative flux (b) for Case 1: uniform temperature of $T = 1000$ K, $f_{\text{H}_2\text{O}} = 1.0$ and $L = 1.0$ m.

considered here, HITEMP1995, to more recent databases of HITRAN2004, HITRAN2008, and HITEMP2010: the results are refined monotonically as an improved spectral database is used. Here we assume that the LBL results from HITEMP2010 are by far the most accurate solution, which is reasonable and logic.

Very good to excellent agreement between the present LBL results using HITEMP2010 and those of the SNB model and the LBL results of Denison [24] is observed from Figs. 2 and 3, suggesting that both the SNB model results using the dataset of Soufiani and Taine [47] and the LBL results of Denison using an extended high resolution spectral database are very accurate under the conditions of Case 1. The results shown in Figs. 2 and 3 indicate that the results of gas radiation are more sensitive to the spectral database or the model at a smaller separation distance, suggesting that the parallel-plate enclosure of a shorter separation distance is a better test case to evaluate the accuracy of a gas radiative property model.

3.2. Isothermal and homogeneous CO_2 (Case 2)

In this case, two sets of conditions of different temperature, CO_2 concentration, and separation distance were considered. LBL calculations were conducted using four high resolution spectral databases, namely HITRAN2004, HITRAN2008, HITEMP2010, and CDSD-1000. The LBL results are compared in Figs. 4 and 5 along with those from the SNB model for the two sets of conditions considered. The LBL results of Denison [24] for the source term distribution are also plotted in Fig. 5(a). From these figures, we

Fig. 4. Distributions of the predicted local radiative source (a) and net radiative flux (b) for Case 2: uniform temperature of $T = 2000$ K, $f_{\text{CO}_2} = 0.5$ and $L = 0.1$ m.

can see that there are significant differences between the LBL results using the two HITRAN databases and those using the HITEMP2010 database for the radiative source term, Figs. 4(a) and 5(a), and the net radiative heat flux, Figs. 4(b) and 5(b). These can be attributed to the missing of hot lines in the HITRAN databases. Bharadwaj and Modest [53] compared the medium resolution transmissivities of CO_2 predicted by CDSD and HITEMP1995 with their experimental measurements and showed that results of the CDSD database were in better agreement with the measured data than those from HITEMP1995. Traditionally, the CDSD database for CO_2 had been more accurate than the HITRAN and HITEMP database prior to the availability of HITEMP2010. Although the differences among the LBL results using HITRAN2004, HITRAN2008, and HITEMP2010 are fairly small for Case 1 shown in Figs. 2 and 3, where the medium contains only H_2O as radiating gas and is at a lower temperature of 1000 K, the corresponding differences are rather large for Case 2, Figs. 4 and 5, where the medium contains CO_2 as the only radiating gas and the temperature is much higher at 2000 K and 1500 K, though the differences between the results of HITRAN2004 and HITRAN2008 are relatively small. These results seem to suggest that the use of HITEMP2010 has a larger influence on calculations of radiation heat transfer due to CO_2 than due to H_2O , compared to use of HITRAN2004 or HITRAN2008. The LBL results calculated using HITEMP2010 and CDSD-1000 (updated) are in excellent agreement, implying that both databases can be used to accurately calculate radiation heat transfer due to

Fig. 5. Distributions of the predicted local radiative source (a) and net radiative flux (b) for Case 2: uniform temperature of $T = 1500$ K, $f_{\text{CO}_2} = 0.1$ and $L = 0.5$ m.

CO_2 . The differences between the present LBL results obtained using either HITEMP2010 or CDS-1000 and the SNB results, Figs. 4 and 5, or the LBL results of Denison [24], Fig. 5(a), can be seen quite small. Such good agreement suggests that the SNB model parameters of Soufiani and Taine [47] and the high resolution spectral database generated in [24] for CO_2 are also quite accurate.

3.3. Isothermal inhomogeneous H_2O (Case 3)

In Case 3 the medium contains an isothermal (at 1000 K) but inhomogeneous $\text{H}_2\text{O}/\text{N}_2$ mixture. As given in Table 2, the H_2O mole fraction is zero near the two plates and 100% in the middle of the enclosure. Fig. 6 displays the distributions of the radiative source term and the net radiative flux calculated using the LBL method and the SNB model for Case 3. The LBL distributions of the source term and the net radiative flux calculated using HITRAN2004 and HITRAN2008 do not differ significantly from each other, especially around the middle of the enclosure, similar to the observations made for Case 1 shown in Figs. 2 and 3. The LBL results using HITEMP2010 exhibit significant differences from those of HITRAN2004 and HITRAN2008, especially for the source term, Fig. 6(a). A comparison between results shown in Figs. 3 and 6 highlights the importance of conducting calculations in inhomogeneous test cases to evaluating the performance of a high-resolution spectral database. Once again, there is excellent agreement between the LBL results using HITEMP2010 and the SNB results in this isothermal and inhomogeneous medium case, which confirms

Fig. 6. Distributions of the predicted local radiative source (a) and net radiative flux (b) for Case 3: parabolic H_2O mole fraction profile, $T = 1000$ K and $L = 1.0$ m.

the finding from Figs. 2 and 3 that the SNB database of Soufiani and Taine [47] for H_2O is very accurate.

3.4. Nonisothermal homogeneous H_2O (Case 4)

In this case the medium consists of nonisothermal pure water vapor. The left plate is hot at 1500 K and the right plate is cool at 300 K. The temperature distribution inside the medium follows a boundary layer type given in [52]. The LBL and SNB results for Case 4 are compared in Fig. 7. It can be seen that there are very small differences among LBL results of different databases or between the LBL results and those of the SNB model. The insensitivity of the LBL results to the spectral databases in this case is unexpected based on the results shown in Fig. 2 for the isothermal case, where the LBL results exhibit a larger sensitivity to the spectral databases considered. The insensitivity of the LBL results to the spectral databases used suggests that Case 4 is not a good choice to evaluate the performance of a spectral database. The SNB results are again in closest agreement with the LBL results using HITEMP2010, Fig. 7(b), further supporting the earlier observations that the SNB database of Soufiani and Taine [47] for H_2O is very accurate.

3.5. One-dimensional air combustion (Case 5)

This case was first considered by Liu et al. [49] to evaluate the performance of a simplified SNB implementation and gray gas models. In this case the medium consists of a nonisothermal and

Fig. 7. Distributions of the predicted local radiative source (a) and net radiative flux (b) for Case 4: boundary layer type temperature profile, $f_{\text{H}_2\text{O}} = 1.0$ and $L = 0.2$ m.

Fig. 8. Distributions of the predicted local radiative source (a) and net radiative flux (b) for Case 5: air combustion scenario, $L = 0.5$ m.

inhomogeneous mixture of $\text{CO}_2/\text{H}_2\text{O}/\text{N}_2$ as shown in Fig. 1. The temperature and mole fraction distributions are typical in a counterflow diffusion flame between a fuel (hydrocarbon) and an air jet. The peak temperature reaches 2000 K at the flame front at $x = 0.14$ m. The distributions of radiative source term and net radiative flux calculated from the LBL and SNB models under this air combustion case are compared in Fig. 8. Due to the fairly low concentrations of CO_2 in this case the CDSD-1000 database was not used in the LBL calculations. It can be seen that the LBL results using HITRAN2004 and HITRAN2008 deviate significantly from those of using HITEMP2010, which is not surprising in this nonisothermal and inhomogeneous case given the fact that many hot-lines are missing from HITRAN2004 and HITRAN2008 at high temperatures beyond about 1000 K. Fig. 8 shows that the agreement between the results of SNB and those of LBL using HITEMP2010 is very good, except the radiative source term around the flame location ($x = 0.14$ m) where the SNB model slightly underestimates the source term. These results once again support the findings that the SNB model parameters of Soufiani and Taine [47] for CO_2 and H_2O are accurate.

3.6. One-dimensional oxy-fuel combustion (Case 6)

Due to the recent interests in oxy-fuel combustion technologies, this case was added in this study. The distributions of temperature

and H_2O mole fraction are the same as those in Case 5. However, CO_2 mole fraction is much higher, as shown in Fig. 1. Due to very high CO_2 mole fractions, it is desirable to include CDSD-1000 database for line properties of CO_2 in LBL calculations. For this purpose, an additional run of LBL calculation was conducted in which the line properties of H_2O were taken from HITEMP2010 while the line properties of CO_2 were from CDSD-1000 (hereafter HITEMP2010 + CDSD-1000). Results for the one dimensional oxy-fuel combustion case are compared in Fig. 9. As expected, the overall trend of the source term and net heat flux distributions is similar to that in the air combustion case shown in Fig. 8. However, the higher concentrations of CO_2 substantially enhance both the source term and the net heat flux. Also similar to the case of air combustion, the LBL results of HITRAN2004 and HITRAN2008 deviate significantly from those of HITEMP2010 for the same reason discussed above. The LBL results calculated using HITEMP2010 and HITEMP2010 + CDSD-1000 are in very good agreement with each other. It is encouraging to see the good agreement between the two different well established high resolution spectral databases for CO_2 , indicating that both databases are capable of providing accurate high resolution spectral information for CO_2 at high temperatures. Like in the air combustion case, the very good agreement between the results of the SNB model and the LBL results calculated using HITEMP2010 is once again observed in Fig. 9, even at the flame location at $x = 0.14$ m.

Fig. 9. Distributions of the predicted local radiative source (a) and net radiative flux (b) for Case 6: oxy-fuel combustion scenario, $L = 0.5$ m.

4. Conclusions

LBL calculations using HITRAN, HITEMP, and CDSD high-resolution spectral databases were conducted for six test cases of radiative heat transfer in one-dimensional enclosure between two parallel plates. These six cases were studied to investigate the relative performance of these databases in isothermal/nonisothermal and homogeneous/inhomogeneous $\text{H}_2\text{O}/\text{N}_2$, CO_2/N_2 , and $\text{CO}_2/\text{H}_2\text{O}/\text{N}_2$ mixtures. The SNB model was also included in the evaluation study with calculations conducted using updated SNB parameters. This study demonstrates the importance of spectral database to the accuracy of LBL calculations through a systematic comparison of LBL results calculated using different databases.

It was found that the LBL results in general show strong dependence to the database used. There exist fairly significant differences between the LBL results using the HITEMP2010 database and those from older databases. HITEMP1995 yields poor results and should not be used for radiative heat transfer calculations. Due to missing of many hot lines HITRAN2004 and HITRAN2008 also should not be used for radiative heat transfer calculations at temperatures above 1000 K. The agreement between the LBL results using HITEMP2010 and CDSD-1000 for Cases 2 and 6 involving CO_2 is very good, which is a good indication that both high resolution spectral databases are accurate and can be used for radiative heat transfer calculations involving CO_2 . The present results of the six test cases suggest that the high-resolution database for high temperature applications, namely, HITEMP2010, is well developed, reliable, and accurate for both H_2O and CO_2 .

The agreement between the LBL results using the HITEMP2010 database and the results of the SNB model was found to be very good for both the wall heat flux and the radiative source term for all the test cases investigated. Very good agreement was also observed between the LBL results using the HITEMP2010 database and the literature LBL results of Denison [24] for the source term distributions in test Cases 1 and 2. Therefore, it can be concluded that the updated SNB parameters are very accurate for both H_2O and CO_2 . This finding has the following important implication: the SNB model along with the updated model parameters is sufficiently accurate to produce benchmark solution for multidimensional radiative heat transfer problems where LBL calculations are infeasible. This finding also supports the practice in the literature to use the SNB model results as benchmark solution whenever LBL results are not available.

The present LBL results using the HITEMP2010 database can serve as benchmark solutions to evaluate the accuracy of other approximate models in the future.

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