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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 CO_2, H_2O, 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 H_2O and CO_2 are accurate. For cases involving CO_2 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.

1. Introduction

Radiative properties of CO_2 and H_2O 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 CO_2 for large-scale and 3D CFD calculations [1,2].

The extremely rapid variation of the radiative properties of real gases (primarily CO_2 and H_2O 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 (W m^{-2} sr^{-1})
I_v	spectral radiation intensity (W m^{-2} sr^{-1} cm^{-1})
k_B	Boltzmann constant (J K^{-1})
$\bar{k}_v$	equivalent mean line-intensity to spacing ratio (cm^{-1} atm^{-1})
L	separation distance between parallel walls (m)
N	molecule number density (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 (cm^{-1} (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 (cm^{-1} atm^{-1})
γ_{self}	self-broadened half-width at 296 K (cm^{-1} atm^{-1})
$\bar{\gamma}_v$	mean half-width of an absorption line (cm^{-1})
$\bar{\delta}_v$	equivalent line spacing (cm^{-1})
Δv	wavenumber interval (cm^{-1})
v	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 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 date 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