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### Abstract

This paper explores the influence of spectral model parameters on the accuracy of the Rank Correlated Spectral Line Weighted-sum-of-gray-gases (RC-SLW) model. The range of the Absorption Line Blackbody Distribution Function (ALBDF) database has been extended as part of this work, and the range of the ALBDF database has been studied as it relates to the RC-SLW model construction and prediction accuracy. The study first defines the maximum lower limit of the absorption cross-section in the ALBDF database which produces accurate predictions of total emissivity. It is shown that although the RC-SLW method yields very good accuracy, results may exhibit some sensitivity to the method used to specify the quadrature bounds. The critical need for sufficiently broad ALBDF data is demonstrated. Complete independence of predictions on blackbody source temperature is demonstrated, provided the solution is sufficiently numerically resolved. Finally, it is shown that accurate predictions may be achieved using the RC-SLW model using just a few gray gases.

**Keywords** gas radiation, spectral model, Rank Correlated SLW method, ALBDF

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“An Exploration of the Influence of Spectral Model Parameters on the Accuracy of the Rank Correlated SLW Model,” by B.W. Webb, V.P. Solovjov, and F. Andre

*Highlights*

1. The influence of spectral model parameters on the predictive accuracy of the Rank Correlated SLW model is explored.
2. The ALBDF database has been re-generated, extending the lower limit of the absorption cross-section to  $10^{-7}$  m<sup>2</sup>/mol.
3. Two methods for specifying the minimum value of the ALBDF in the model spectral construction are proposed, with an investigation of the attendant assumptions needed.
4. It is demonstrated that if sufficient numerical resolution is used the model predictions are independent of the specified value of the blackbody source temperature.
5. It appears that optimal predictive accuracy with the fewest gray gases is achieved when the spatial average temperature is selected as the blackbody source temperature.

# AN EXPLORATION OF THE INFLUENCE OF SPECTRAL MODEL PARAMETERS ON THE ACCURACY OF THE RANK CORRELATED SLW MODEL

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**ABSTRACT** This paper explores the influence of spectral model parameters on the accuracy of the Rank Correlated Spectral Line Weighted-sum-of-gray-gases (RC-SLW) model. The range of the Absorption Line Blackbody Distribution Function (ALBDF) database has been extended as part of this work, and the range of the ALBDF database has been studied as it relates to the RC-SLW model construction and prediction accuracy. The study first defines the maximum lower limit of the absorption cross-section in the ALBDF database which produces accurate predictions of total emissivity. It is shown that although the RC-SLW method yields very good accuracy, results may exhibit some sensitivity to the method used to specify the quadrature bounds. The critical need for sufficiently broad ALBDF data is demonstrated. Complete independence of predictions on blackbody source temperature is demonstrated, provided the solution is sufficiently numerically resolved. Finally, it is shown that accurate predictions may be achieved using the RC-SLW model using just a few gray gases.

## *Keywords*

gas radiation, spectral model, Rank Correlated SLW method, ALBDF

## INTRODUCTION

The absorption characteristics of gases are extraordinarily complex [1], which makes prediction of radiative transfer in such situations challenging. The last two decades have seen significant progress in the development of engineering approaches for the prediction of radiative transfer in high temperature gases. So-called global approaches, including the Spectral Line Weighted-sum-of-gray-gases (SLW), Full Spectrum  $k$ -distribution (FSK), and Absorption Distribution Function (ADF) models have been developed to enable efficient calculation of radiative transfer [2-5]. The SLW and FSK methods, which are equivalent in isothermal, homogeneous systems [2-4], have been shown theoretically to approach line-by-line accuracy at a small fraction of the cost of line-by-line predictions [6]. These models have been extended to scenarios involving non-isothermal and non-homogeneous media, gas mixtures, and particulates. Significant supporting work has gone into the development of compact databases for capturing the spectral nature of the gas absorption. One such database used in the SLW model, the Absorption-line Blackbody Distribution Function (ALBDF), has been generated for H<sub>2</sub>O, CO<sub>2</sub>, and CO for a wide range of temperature, mole fraction (where appropriate), and total pressure [7].

The treatment of radiation transfer in non-isothermal, non-homogeneous gas media is challenging due to the spatial variation of the thermodynamic states in the domain, and the complexities of accounting for the corresponding radical variations in local spectral absorption properties. The general approach in dealing with these spatial variations in gas absorption spectrum is to invoke a correlated or scaled spectrum assumption, with spectra being “corrected” from a reference spectrum corresponding to a reference thermodynamic state in the domain. This requires the specification of a reference thermodynamic state. This general approach has been extensively demonstrated in the traditional framework of the SLW model [3]. A recent publication presented a family of SLW models for non-uniform media, each with its unique approach and implications for predictive accuracy [8]. One model among these has proved to be a significant advance in the area. The Rank Correlated SLW (RC-SLW) model offers greater simplicity in its spectral construction,

requires only two distribution functions to effect the spectral correlation, and perhaps most importantly, does not require the specification of a reference gas thermodynamic state. In sample predictions the RC-SLW model showed accurate predictions with relatively few gray gases.

This paper explores the sensitivity of input parameters on predictions using the Rank Correlated SLW model. The paper briefly reviews the spectral construction of the RC-SLW model, and discusses the parameters and data required for the prediction of radiative transfer using the model. The sensitivity of predictions to spectral parameters is explored in some depth for the method.

### CONSTRUCTION OF THE RANK CORRELATED SLW SPECTRAL MODEL

The detailed theoretical development of the assumption of rank correlation of the gas absorption spectrum, and the corresponding development of the Rank Correlated SLW (RC-SLW) model can be found elsewhere [8, 9]. Notably, despite assuming a correlated spectrum the Rank Correlated SLW model for prediction of radiative transfer in non-uniform media does not require specification of any gas reference thermodynamic state for its construction. The method will be briefly outlined here.

Propagation of radiation in absorbing and emitting gaseous media along a pathlength  $s$  in a direction  $\mathbf{\Omega}$  is characterized by the spectral radiation intensity  $I_\eta(s, \mathbf{\Omega})$ , which is governed by the Radiative Transfer Equation (RTE):

$$\frac{\partial I_\eta(s, \mathbf{\Omega})}{\partial s} = -\kappa_\eta(s) I_\eta(s, \mathbf{\Omega}) + \kappa_\eta(s) I_{b\eta}[T(s)] \quad (1)$$

The gray-gas form of the RTE may be written as

$$\frac{\partial I_j(s, \mathbf{\Omega})}{\partial s} = -\kappa_j(s) I_j(s, \mathbf{\Omega}) + a_j \kappa_j(s) I_b[T(s)] \quad (2)$$

The objective in the Spectral Line Weighted-sum-of-gray-gases (SLW) model is to find the local values of the gray gas absorption coefficients  $\kappa_j$  and the corresponding gray gas weights  $a_j$ . The RTE Eq. (2) is then solved for each gray gas, and the total intensity is found by summing over all

gray gases. Thus, the method replaces an integration over wavenumber as in the line-by-line method with an integration over absorption cross-section (or absorption coefficient).

The basis for representing the complex spectral absorption data in compact form in the SLW model is the Absorption Line Blackbody Distribution Function (ALBDF). For a gas at a given thermodynamic state  $\phi_g$  (temperature, mole fraction, total pressure) and a given blackbody source temperature  $T_b$ , the ALBDF  $F(C, \phi_g, T_b)$  of the absorption cross-section  $C$  describes the fraction of the total blackbody radiative power  $E_b(T_b) = \sigma T_b^4$  emitted at temperature  $T_b$  that lies in the part of the spectrum where the spectral absorption cross-section  $C_\eta(\phi_g)$  is below a prescribed value  $C$ . The ALBDF is defined mathematically as follows:

$$F(C, \phi_g, T_b) = \frac{I}{E_b(T_b)} \int_{\{\eta: C_\eta(\phi_g) < C\}} E_{b\eta}(T_b) d\eta = \int_0^\infty H(C - C_\eta(\phi)) \frac{E_{b\eta}(T_b)}{E_b(T_b)} d\eta \quad (3)$$

Here,  $H$  is the Heaviside unit-step function. The ALBDF is a strictly increasing function varying between 0 and 1 in the variable  $C$ , and therefore, it is invertible. The inverse ALBDF  $C(F, T_g, T_b)$  of the variable  $F$  is defined such that

$$C[F(C, \phi_g, T_b), \phi_g, T_b] = C \text{ and } F[C(F, \phi_g, T_b), \phi_g, T_b] = F \quad (4)$$

The inverse ALBDF can be interpreted as a reordered gas absorption cross-section.

The construction of the RC-SLW spectral model is rather simple, and is illustrated schematically in Fig. 1. The starting point is a subdivision of the ALBDF  $F$ -variable into two sets of discrete supplemental values  $0 \leq F_{\min} \leq \tilde{F}_j \leq F_{\max} \leq 1$  for  $j = 0, 1, 2, \dots, n$  and  $\tilde{F}_{j-1} \leq F_j \leq \tilde{F}_j$  for  $j = 1, 2, \dots, n$  (as shown on the left-hand side of the abscissa in Fig. 1), where  $n$  is the number of gray gases in the model. The corresponding local supplemental values of absorption cross-section (shown on the ordinate of Fig. 1) are then calculated by

$$\tilde{C}_j^{loc} = C(\tilde{F}_j, \phi_{loc}, T_b) \text{ for } j = 0, 1, 2, \dots, n \quad (5)$$

and

$$C_j^{loc} = C(F_j, \phi_{loc}, T_b) \text{ for } j = 1, 2, \dots, n \quad (6)$$

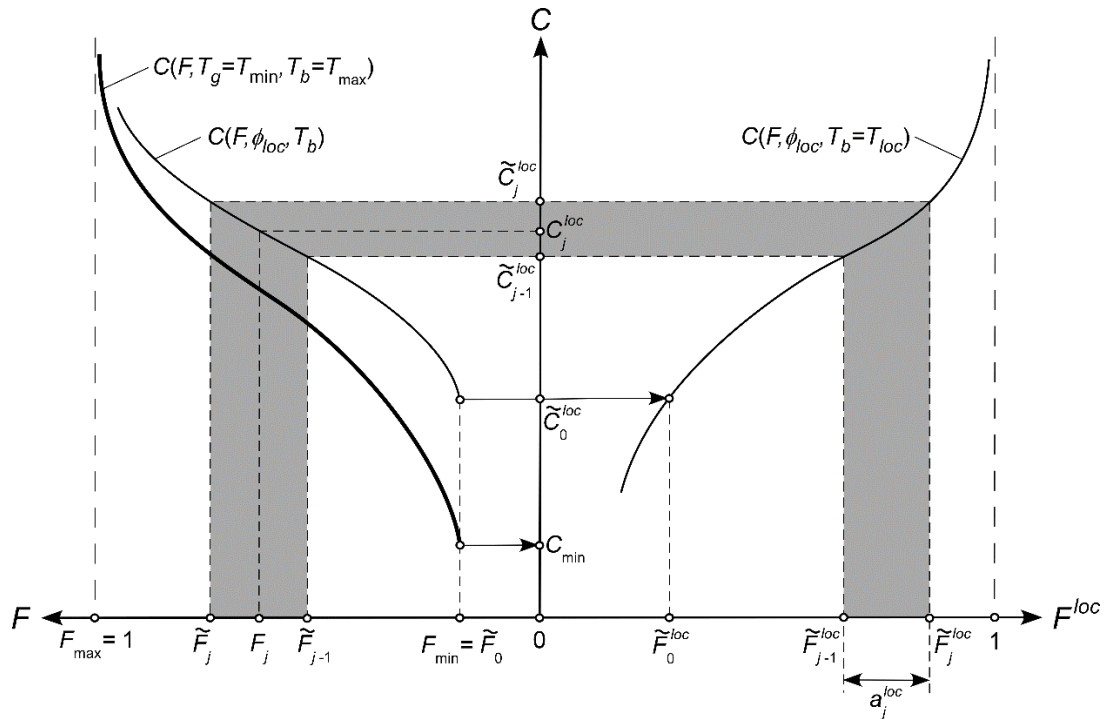


Figure 1. Graphical illustration of the construction of the Rank Correlated SLW spectral model.

It is assumed implicitly that as the number of gray gases,  $n$ , is increased the accuracy of the RC-SLW model predictions will improve, and that the error will reach an unchanging value with increasing  $n$ . That limiting error is defined by the approximations inherent in the modeling approach. The dependence of model predictions on the number of gray gases will be a part of the exploration here.

In the development of the RC-SLW spectral model the blackbody source temperature  $T_b$  is fixed, subject to the assumption of rank correlation of the spectral absorption cross-section at different thermodynamic states. This eliminates the appearance of undesirable Leibnitz terms in the spectrally integrated RTE [8]. As has been previously suggested [9,10], the blackbody source temperature is merely a mathematical convenience, and theoretically, predictions should be independent of the value of  $T_b$  selected. This presumption is explored here.



The gray gas absorption coefficients corresponding to the local absorption cross-sections are  $\kappa_j^{loc} = N^{loc} C_j^{loc}$ , and the local gray gas weights may then be calculated as (shown on the right-hand side of the abscissa in Fig. 1)

$$a_j^{loc} = \tilde{F}^{loc}(\tilde{C}_j^{loc}, \phi_{loc}, T_{loc}) - \tilde{F}^{loc}(\tilde{C}_{j-1}^{loc}, \phi_{loc}, T_{loc}) = \tilde{F}_j^{loc} - \tilde{F}_{j-1}^{loc} \quad (7)$$

The local weight of the clear gas, for which  $\kappa_0 = 0$ , is calculated as

$$a_0^{loc} = \tilde{F}^{loc}(\tilde{C}_0^{loc}, \phi_{loc}, T_{loc}) = \tilde{F}_0^{loc} \quad (8)$$

**Spectral Windows** The spectral windows in the RC-SLW model warrant special discussion. The value of the zeroth supplemental cross-section is stated as

$$\tilde{C}_0^{loc} = C(F_{\min}, \phi_{loc}, T_b) \quad (9)$$

This defines the spectral windows (transparent spectral intervals, otherwise known as clear gas) of the absorption cross-section  $\Delta_0^{loc} = \{\eta : C_\eta(\phi_{loc}) < \tilde{C}_0^{loc}\}$  for the SLW model. It is in these spectral windows that the absorption cross-section (and correspondingly, absorption coefficient) vanish. As explained by Hottel [11], the spectral windows are necessary for proper weighted-sum-of-gray-gases (WSGG) modelling of gas radiation. In the WSGG modelling of a gas layer of thickness  $L$  the total emissivity is expressed as

$$\varepsilon = \sum_{j=1}^n a_j (1 - e^{-\kappa_j L}) \quad (10)$$

In a weighted-sum-of-gray gases model that does not include a clear gas, *i.e.*, where  $\kappa_j > 0$  and where the weights sum to unity (for  $j = 1$  to  $n$ ), the gas total emissivity will increase as the path-length  $L$  is increased, reaching a value  $\varepsilon = 1$  at unrealistic values of  $L$ . In reality, the true behavior of the emissivity as  $L \rightarrow \infty$  will depend critically on the rigorous accounting of all spectral lines (even beyond what may be found in current spectroscopic databases), the inclusion of all relevant lines in the database, and the treatment of line wings (which is, even today, somewhat arbitrary).

As shown by Eq. (10), in a weighted-sum-of-gray-gases model with appropriate spectral windows, as  $L \rightarrow \infty$  the total emissivity becomes

$$\lim_{L \rightarrow \infty} \varepsilon = \sum_{j=1}^{\infty} a_j = 1 - a_0 \quad (11)$$

where  $a_0$  is the weight of the clear gas,  $j = 0$ . Thus, the proper definition of the transparency intervals is essential in weighted-sum-of-gray-gases modelling of radiative transfer in high temperature gases for pathlengths of engineering relevance.

**Determination of Gray Gas Absorption Coefficients and Weights** Subdivision into gray gases by discretization of the corresponding  $F$ -variable in the interval  $0 \leq F_{\min} \leq \tilde{F}_j \leq F_{\max} \leq 1$  is arbitrary in the RC-SLW model. In a modeling scenario with a large number of gray gases, even simple uniform subdivision is likely satisfactory for accurate results. If, however, a small number of gray gases is used a more efficient subdivision can be obtained by using Gauss-Legendre integral quadrature nodes and weights, which will accentuate higher values of gas absorption cross-section. The  $F$ -variable is then subdivided into supplemental values of the ALBDF ( $\tilde{F}$ ) by mapping of Gauss-Legendre quadratures from the  $x$ -interval  $[0, 1]$  to the  $F$ -interval  $[F_{\min}, F_{\max}]$  as follows:

$$\tilde{F}_j = F_{\min} + (F_{\max} - F_{\min}) \sum_{k=1}^j w_k \quad \text{for } j = 1, 2, \dots, n \quad (12a)$$

$$F_j = F_{\min} + (F_{\max} - F_{\min}) x_j \quad \text{for } j = 1, 2, \dots, n \quad (12b)$$

and

$$\tilde{F}_0 = F_{\min} \quad (12c)$$

where  $x_j$  and  $w_j$  are the nodes and corresponding weights, respectively, of the quadrature in the  $x$ -interval  $[0, 1]$ , and where the values of  $F_j$  are also transformed to the quadrature nodes  $x_j$ . The local values of absorption cross-section (and corresponding gray gas absorption coefficient) and

gray gas weights are found (assuming fixed blackbody source temperature  $T_b$ ) from Eqs. (5-8), where  $\kappa_j^{loc} = N^{loc} C_j^{loc}$ .

**Generation of the ALBDF** The ALBDF,  $F(C, \phi_g, T_b)$ , is generated from the detailed gas absorption spectrum at a given gas thermodynamic state  $\phi_g$  and for a specified blackbody source temperature  $T_b$ . The maximum value of absorption cross-section used as upper bound in the generation of the ALBDF is selected so as to practically capture the peaks in the thousands (perhaps millions) of absorption lines. Pearson *et al.* [7] have presented ALBDF data in both mathematical correlation (hyperbolic tangent) and tabulated data (lookup table) form. A maximum value  $C_{max} = 10^3$  m<sup>2</sup>/mol was used in the generation of the ALBDF, which, for practical purposes at all gas thermodynamic conditions of engineering relevance yields  $F_{max} = F(C_{max}, \phi_g, T_b) = 1.0$  for H<sub>2</sub>O, CO<sub>2</sub>, and CO. At the lower bound of  $C$  in the assembly of the ALBDF, it is neither necessary nor wise to generate the ALBDF from the detailed gas absorption spectrum for vanishing values of the absorption cross-section,  $C \rightarrow 0$ . Generally, the absorption spectrum can be confidently assumed to be effectively transparent below a specified finite value of absorption cross-section,  $C_{min}$ , and this value thus represents a practical lower bound in the generation of the ALBDF. Denison and Webb used a minimum value  $C_{min} = 3 \times 10^{-5}$  m<sup>2</sup>/mol in the generation of ALBDF empirical correlations [12], whereas Pearson *et al.* [7] more recently adopted the value  $C_{min} = 10^{-4}$  m<sup>2</sup>/mol for both empirical correlations and tabulated ALBDF data. The values of  $C_{min}$  and  $C_{max}$  used in the previous databases have been shown to yield very good accuracy in a wide range of problems. As part of this investigation the ALBDF database was re-generated from the detailed absorption spectrum of Pearson *et al.* using a value of  $C_{min} = 10^{-7}$  m<sup>2</sup>/mol, which is three decades lower than that used previously by Pearson *et al.* [7]. It should be mentioned that the value  $C_{min} = 10^{-7}$  m<sup>2</sup>/mol is well above the absorption line cutoff of  $6.0 \times 10^{-10}$  m<sup>2</sup>/mol used by Pearson in summing the contri-

bution of adjacent absorption lines at a given wavenumber in the assembly of the detailed absorption spectrum. The dependence of the RC-SLW model’s accuracy on the value of  $C_{\min}$  will be investigated in detail here by comparing model predictions with line-by-line calculations.

There are some technical issues in construction of the spectral model as it relates to the ALBDF data that bear exploring here. The first step in the RC-SLW spectral model is the discretization of the  $F$ -variable. The choice of the minimum value  $F_{\min}$  in this discretization is important for efficient and accurate predictions. It might be argued that  $F_{\min}$  should always be set to zero. However, this may not be a wise use of a limited number of gray gases, since low values of  $F$  in the model calculations may yield corresponding values of  $\tilde{C}_j^{loc} = C(\tilde{F}_j, \phi_{loc}, T_b)$  in the model which lie below the value of  $C_{\min}$  used in the generation of the ALBDF database. In other words, for a given  $F_{\min}$ , some gas thermodynamic states may yield values of  $F$  which correspond to  $\tilde{C}_j^{loc}$  below the minimum value  $C_{\min}$  in the ALBDF database. While this is not an inherent limitation in the RC-SLW model, it does illustrate the dependence of the model’s accuracy on the extent of the ALBDF database.

Given the practical (but previously demonstrated reasonable and accurate) limits in the ALBDF database an approximate treatment is needed for scenarios where  $\tilde{C}_j^{loc} = C(\tilde{F}_j, \phi_{loc}, T_b)$  may fall below the ALBDF minimum database value of  $C_{\min}$ . One approach might be to extrapolate the ALBDF to values below  $C_{\min}$  for which the ALBDF has been tabulated (or correlated). Unfortunately, it is not clear how to perform this extrapolation due to the fact that the ALBDF is often not well-behaved at low values of  $C$ . Alternatively, given that it is assumed that the gas absorption spectrum is transparent below the value of  $C_{\min}$  used to generate the ALBDF, it is not unreasonable to assume that for all values of  $\tilde{C}_j^{loc} = C(\tilde{F}_j, \phi_{loc}, T_b)$  that fall below  $C_{\min}$ , the absorption cross-section vanishes. This, however, has the potential to result in artificially high gray gas weights associated with these low values of  $\tilde{C}_j^{loc}$  because the values of  $\tilde{C}_j^{loc}$  which straddle  $C_{\min}$  (inside and outside the domain of the ALBDF database) may result in correspondingly high differences in  $F_j^{loc}$ , leading to erroneously large gray gas weights.

The approximation adopted here in the case of  $\tilde{C}_j^{loc}$  falling below  $C_{\min}$  in the ALBDF database is the following. If  $\tilde{C}_j^{loc} < C_{\min}$ , then  $\tilde{C}_j^{loc}$  is assigned to be equal to  $C_{\min}$ , which forces zero gray gas weights for these low values of  $\tilde{C}_j^{loc}$ . The justification for this approximation is that the influence of gray gases on the radiative transfer calculations presumably diminish as  $C \rightarrow 0$ . Thus, it seems reasonable to assume the weights of these gray gases vanish. In effect, this forces these gray gases below  $C_{\min}$  to be transparent, consistent with the assumption that the spectrum is transparent for the corresponding spectral regions. It must be acknowledged that this assumption may have the undesirable effect of eliminating gray gases with low but finite absorption coefficient in the model that will contribute to the radiative transfer (perhaps more important particularly at increasingly large pathlengths), potentially leading to inaccuracy in the predictions. This will be investigated as part of this work.

Given all of these considerations, it may be desirable to choose a value of  $F_{\min}$  as a compromise.  $F_{\min}$  might be chosen high enough such that *i*) any local thermodynamic state  $\tilde{C}_j^{loc}$  will not fall below the minimum value of absorption cross-section  $C_{\min}$  in the tabulated ALBDF data, and *ii*) a finite number of gray gases is deployed efficiently between  $F_{\min}$  and  $F_{\max}$ . However,  $F_{\min}$  should not be chosen so high as to artificially exaggerate the transparency intervals, effectively excluding participating spectral lines from the model predictions. These considerations for the selection of  $F_{\min}$  are thus influenced both by the RC-SLW model construction and the extent of the ALBDF database (*i.e.*, the value of  $C_{\min}$  used in the generation of the database).

Analysis of the ALBDF  $F(C, T_g, T_b)$  behavior reveals it to be monotonically increasing with both decreasing gas temperature  $T_g$  and increasing blackbody source temperature  $T_b$  [7, 12]. This suggests that an optimal choice of  $F_{\min}$  may be

$$F_{\min} = F(C = C_{\min}, T_g = T_{\min}, T_b = T_{\max}) \quad (13)$$

where  $T_{\max}$  and  $T_{\min}$  are the maximum and the minimum gas temperature in the system and  $C_{\min}$  is the minimum value of  $C$  used in the representation of ALBDF data. Adopting this choice of  $F_{\min}$

based on the prescribed value of  $C_{\min}$ , it can be seen in Fig. 1 that for all possible gas thermodynamic states in the domain the calculated value of  $F$  will be above  $F_{\min}$ . At any local gas temperature the local absorption cross-sections calculated in the RC-SLW model are then guaranteed to lie in the domain of the ALBDF data,  $\tilde{C}_j^{loc} \geq C_{\min}$ , and no approximation of the ALBDF is needed. However, the predictive accuracy of this specification of  $F_{\min}$  depends intimately on the extent of the ALBDF database, since  $F_{\min}$  calculated using Eq. (13) depends on  $C_{\min}$ . Further, while this calculation of  $F_{\min}$  ensures that all values of  $\tilde{C}^{loc}$  lie within the domain of the ALBDF database used, it can, in some cases, result in unrealistically high values of  $F_{\min}$ , depending on the value of  $C_{\min}$  used. At some gas thermodynamic states  $\phi_g$ , and for some values of blackbody source temperature  $T_b$ , the value  $C_{\min} = 10^{-4} \text{ m}^2/\text{mol}$  used previously by Pearson *et al.* to generate the ALBDF database [7] produces a very wide range of the corresponding values of  $F_{\min}$  in the calculation of Eq. (13)—from as low as 0.1 to as high as 0.8. Determining  $F_{\min}$  according to Eq. (13) thus has the possibility of restricting the radiative transfer calculations in the RC-SLW model to very high values of  $F$ . As stated previously, this may have the undesirable effect of excluding significant spectral content from the radiative transfer calculations. This will be investigated in example predictions to follow.

In summary, it is clear that the accuracy of a prediction using the RC-SLW model can depend on a number of parameters in the spectral construction of the model and its implementation. Specifically, the following parameters will be explored in regards to their influence on RC-SLW model predictive accuracy:

1. The extent of the ALBDF database, principally prescribed by  $C_{\min}$  and  $C_{\max}$  used in the generation of the database;
2. The values selected for  $F_{\min}$  and  $F_{\max}$  in the discretization constituting the first step of the model construction, and the assumptions that may be required as a result of selections made;
3. The value of the blackbody source temperature used,  $T_b$ ; and

4. The number of gray gases used in the numerical solution,  $n$ .

It will be shown hereafter that the effect of these model parameters on accuracy is sometimes mutually dependent. The interdependencies will be investigated hereafter in an effort to identify the parameters for optimal model accuracy.

## RESULTS AND DISCUSSION

The accuracy of the ALBDF lookup table is first investigated by calculating gas emissivity using all tabulated values in the table. This exercise is done independent of the RC-SLW model to explore the accuracy of the ALBDF database as a function of  $C_{\min}$  (*i.e.*, the spectral extent of the database). Figure 2 illustrates the predicted emissivity and error in emissivity for CO<sub>2</sub> and H<sub>2</sub>O (for  $Y = 1.0$ ) at  $T_g = 2500$  K (an extreme temperature for which errors will be greatest) for a path-length range  $L = 10^{-2}$  to  $10^7$  m. The unrealistically extreme upper limit on pathlength is chosen simply to illustrate the value of  $C_{\min}$  for which the predicted emissivity departs from the LBL benchmark as the pathlength increases. The figure shows emissivity *i*) calculated from the detailed absorption spectrum using a rigorous line-by-line approach, and *ii*) calculated according to Eq. (10) using all data available in the ALBDF lookup table for the selected value of  $C_{\min}$ , in the range  $10^{-7}$  to  $10^{-2}$  m<sup>2</sup>/mol.

The data of Fig. 2 reveal generally that the emissivity predicted from the ALBDF lookup table matches the LBL benchmark at low values of  $C_{\min}$  but departs from the benchmark at some path-length. The pathlength at which error first appears decreases at higher values of  $C_{\min}$ . The error in emissivity thus increases as either  $L$  or  $C_{\min}$  increase, resulting from the increasing importance of absorption line wings at larger  $L$  and the loss of spectral content in the ALBDF database as  $C_{\min}$  is increased. The error in predicted emissivity is observed to be negligibly small for both CO<sub>2</sub> and H<sub>2</sub>O for all values of  $L$  (even at the extreme pathlengths shown) for  $C_{\min} = 10^{-7}$  m<sup>2</sup>/mol, the value used in the ALBDF data re-generated as part of this study. Further, Fig. 2 shows that the emissivity asymptotes to  $1 - a_0$  as  $L \rightarrow \infty$ , where  $a_0$  is the weight of the clear gas in the SLW model for the

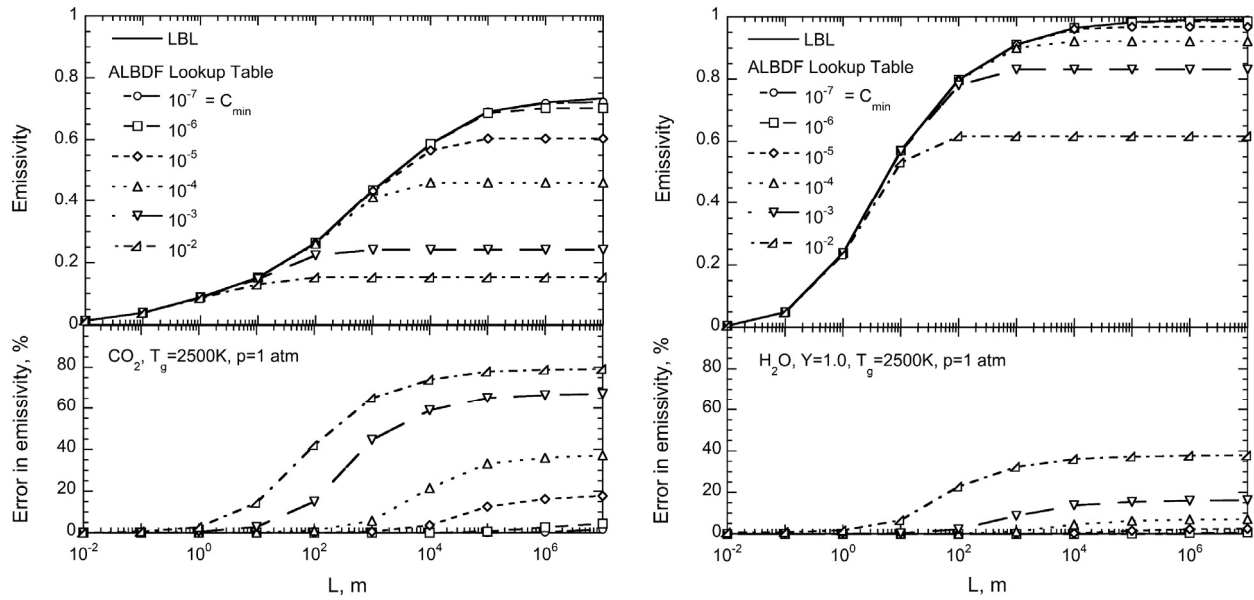


Figure 2. Predicted emissivity and error in emissivity as a function of pathlength  $L$  and  $C_{\min}$  for  $\text{CO}_2$  and  $\text{H}_2\text{O}$  ( $Y = 1.0$ ) at  $T_g = 2500$  K.

particular value of  $C_{\min}$  used. Finally, the data of Fig. 2 show that for a range of pathlength  $L < 100$  m of practical engineering interest the error in emissivity is negligible for  $C_{\min} \leq 10^{-5} \text{ m}^2/\text{mol}$ . These data suggest that the ALBDF lookup table can be confidently used for accurate fundamental absorption/emission characteristics for any radiation pathlength of practical engineering interest with  $C_{\min} \leq 10^{-5} \text{ m}^2/\text{mol}$ .

### Example Problem

Consider radiative transfer in a one-dimensional plane layer of thickness  $L$  bounded by black walls and containing a non-isothermal, non-homogeneous mixture of  $\text{H}_2\text{O}$  and  $\text{CO}_2$ , as studied previously [13]. The temperature and concentration profiles are given by

$$T(x) = 4\Delta T x(L-x)/L^2 + 800, \text{ K} \quad (14a)$$

$$Y_{\text{H}_2\text{O}}(x) = 0.8x(L-x)/L^2 + 0.12 \quad (14b)$$

$$Y_{\text{CO}_2}(x) = 0.4x(L-x)/L^2 + 0.06 \quad (14c)$$



where  $\Delta T = T_{\max} - T_{\min}$ . The ratio of gas mole fractions, H<sub>2</sub>O and CO<sub>2</sub>, is spatially constant for this example at  $Y_{\text{H}_2\text{O}}/Y_{\text{CO}_2} = 2$ . Three different cases for the gas layer thickness are considered in this example problem,  $L = 0.1, 1.0, \text{ and } 5.0$  m. The maximum temperature in the gas layer,  $T_{\max}$ , occurs at the middle point of the layer, and in all cases the minimum temperature,  $T_{\min} = T_0 = T_L = 800$  K, is at the walls. Two different gas temperature ranges are explored corresponding to  $T_{\max} = 1800$  K and 2800 K, for which the maximum temperature differences in the layer are  $\Delta T = 1000$  K and 2000 K, respectively. The average gas temperature of the layer for the two temperature ranges is, respectively,  $T_{\text{ave}} = 1467$  K and  $T_{\text{ave}} = 2133$  K. This set of layer thicknesses and temperature ranges permits the exploration of RC-SLW model parameters for a broad range of optical depth, temperature difference (and corresponding gas absorption spectrum), and temperature gradient.

Prediction of the total divergence of the net radiative flux is performed using the analytical multilayer solution [14] applied to the Rank Correlated SLW model using a variable number of gray gases between  $n = 2$  and 25. A spatial resolution of 100 incremental spatial layers in the domain was used. The mixture of H<sub>2</sub>O and CO<sub>2</sub> in the RC-SLW method is treated as a single gas using the SLW Multiplication Approach described in [15]. The newly generated ALBDF database using a smaller value of absorption cross-section,  $C_{\min} = 10^{-7}$  m<sup>2</sup>/mol, has been used in the simulations. However, the influence of  $C_{\min}$  on the predictions is investigated parametrically by systematically specifying values of  $C_{\min}$  higher than that which was used to build the database (*i.e.*,  $C_{\min} > 10^{-7}$  m<sup>2</sup>/mol), thus truncating the ALBDF data as though the ALBDF had been generated with higher values of  $C_{\min}$ .

Line-by-line (LBL) benchmark predictions were performed with the same multilayer analytical solution as that employed in the RC-SLW method solution, with spectral integrations performed using a summation over all spectral intervals. Again, 100 incremental spatial layers were used in the multilayer LBL solution. The high-resolution gas absorption spectra based on the HITEMP2010 [16] spectral database for H<sub>2</sub>O, and the CDSD-4000 [17] database for CO<sub>2</sub> were used with spectral wavenumber discretization  $\Delta\eta = 0.01$  cm<sup>-1</sup>. More details about these spectral

databases can be found in [18]. Detailed comparisons, not reported here, have shown that the use of the CDSD-4000 database instead of HITEMP2010 for CO<sub>2</sub> in the construction of the SLW model database does not provide significant differences in full spectrum radiative transfer predictions at these temperatures.

Two approaches are used in the exploration of the dependence of spectral model parameters on the accuracy of the RC-SLW model, and particularly the range of  $F$  used in the discretization and integration. The first is to set  $F_{\min} = 0$ , and the second is to calculate  $F_{\min}$  using Eq. (13). The influence of  $C_{\min}$  is investigated in both approaches by systematically raising the minimum value of  $C_{\min}$  used in the predictions above  $C_{\min} = 10^{-7}$  m<sup>2</sup>/mol used in the re-generation of the ALBDF database here, thus artificially truncating the ALBDF database.

For evaluation and quantitative comparison of the accuracy of the RC-SLW model predictions and the dependence on input parameters, the local absolute relative error,  $LE$ , and total absolute relative error,  $TE$ , in prediction of the total divergence of the local net radiative flux  $Q$  are presented using a definition proposed previously [13]:

$$LE(x) = \left| \frac{Q_{SLW}(x) - Q_{LBL}(x)}{\max |Q_{LBL}(x)|} \right|, \% \quad (15)$$

and

$$TE = \frac{\int_0^L |Q_{SLW}(x) - Q_{LBL}(x)| dx}{\int_0^L |Q_{LBL}(x)| dx}, \% \quad (16)$$

The RC-SLW spectral model construction and dependence of predictions on the ALBDF database is now explored. Figure 3 illustrates the value of  $F_{\min}$  calculated according to Eq. (13) shown as a function of  $C_{\min}$  for the two temperature ranges studied here, 800 – 1800 K and 800 – 2800 K. It should be noted that the value of  $F_{\min}$  calculated is a function only of the spectral construction of the RC-SLW model, and not the layer thickness or the number of gray gases used. Figure 3 shows that the value of  $F_{\min} \rightarrow 0$  for both temperature ranges as  $C_{\min} \rightarrow 0$ . Further, it is seen that  $F_{\min}$  calculated according to Eq. (13) increases with increasing  $C_{\min}$ , and can reach very high values—greater than  $F_{\min} = 0.8$  for  $C_{\min} = 10^{-2}$  m<sup>2</sup>/mol at the higher temperature range. At

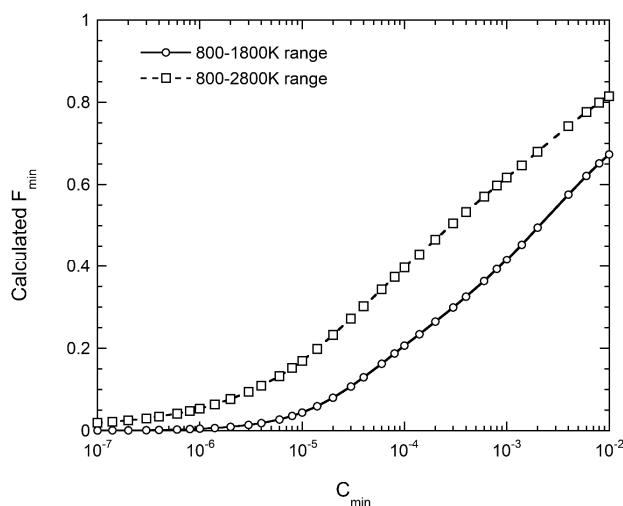


Figure 3.  $F_{\min}$  calculated as a function of  $C_{\min}$  according to Eq. (13) for the two temperature ranges studied.

the value of  $C_{\min}$  used previously in the generation of the ALBDF by Pearson *et al.* [7] ( $C_{\min} = 10^{-4} \text{ m}^2/\text{mol}$ ) the calculated value of  $F_{\min}$  is quite large, and is even larger for the higher temperature range. As was observed previously, a value of  $F_{\min}$  that is too high can result in the exclusion of significant spectral content in the radiative transfer prediction, and will be seen in predictions to follow.

Figure 4 shows the dependence of the total absolute relative error,  $TE$ , in the predictions as a function of  $C_{\min}$  for the three layer thicknesses and the two temperature ranges investigated. In all cases three different blackbody source temperatures were used,  $T_b = T_{\min}$ ,  $T_b = T_{\text{ave}}$ , and  $T_b = T_{\max}$ , where the minimum temperature for both ranges is 800 K, the average temperatures for the two ranges is 1466 K and 2133 K, and the maximum temperatures are 1800 K and 2800 K. Not surprisingly, the predictions show that the error generally increases with an increase in  $C_{\min}$  for all values of  $T_b$ . This is due to the fact that higher  $C_{\min}$  results in more spectral information being excluded from the calculation. Figure 4 also shows that the total error for all cases is asymptotic for  $C_{\min} \rightarrow 0$ . The error is generally higher as the layer thickness increases, perhaps due to the fact that weaker spectral lines have a greater influence as the optical pathlength increases. At  $C_{\min} = 10^{-7} \text{ m}^2/\text{mol}$  the accuracy is sometimes better with  $F_{\min} = 0$  and sometimes with  $F_{\min}$  calculated

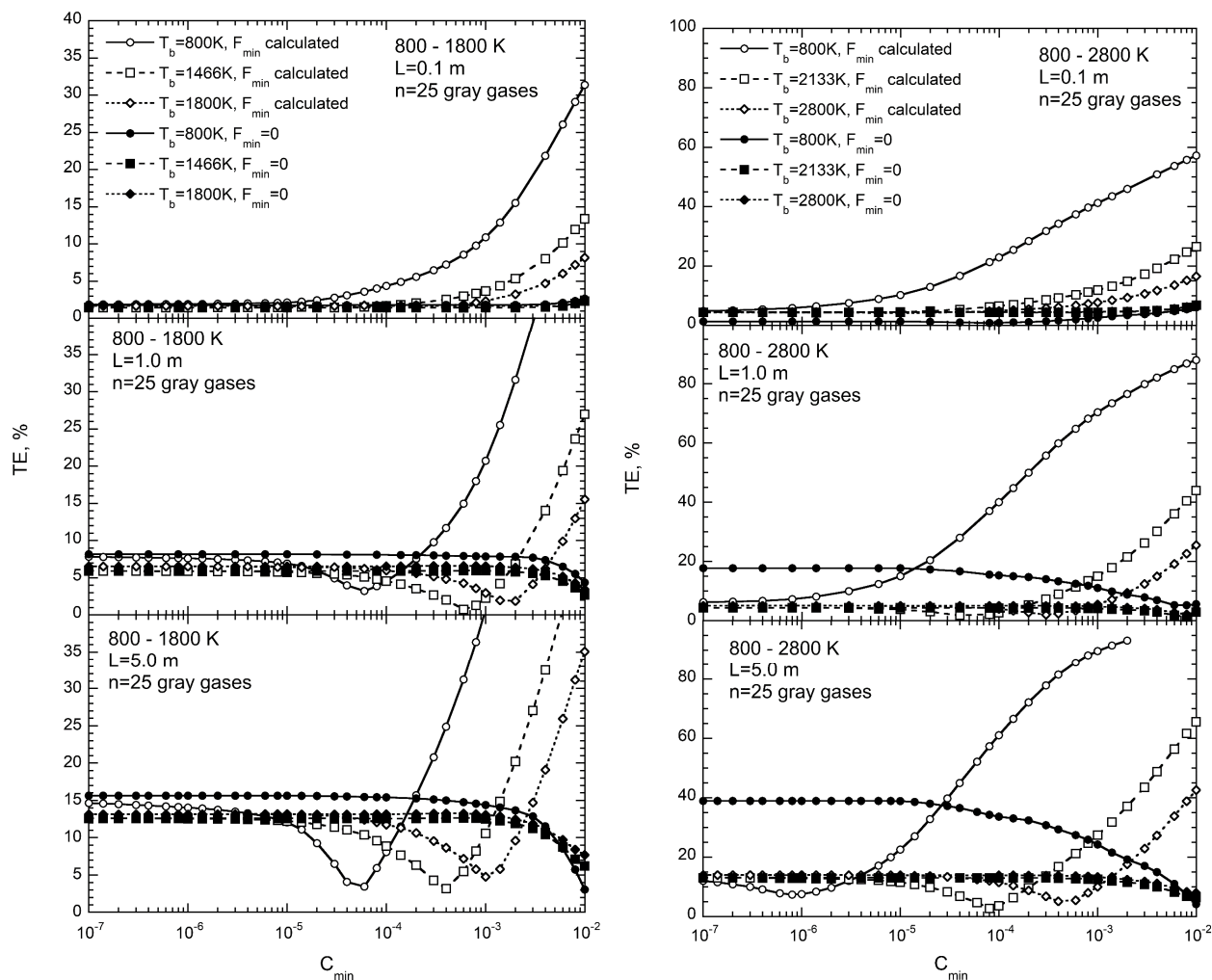


Figure 4. Dependence of the total absolute relative error on  $C_{\min}$  and  $T_b$  for the three layer thicknesses and two temperature ranges investigated for  $F_{\min}$  calculated according to Eq. (13) and  $F_{\min} = 0$ . The number of gray gases used is  $n = 25$ .

from Eq. (13), although the difference in predicted total error for the two methods is modest since  $F_{\min}$  calculated according to Eq. (13) is nearly zero for  $C_{\min} = 10^{-7} \text{ m}^2/\text{mol}$ . Figure 4 also suggests that when  $F_{\min}$  is calculated according to Eq. (13), the error is significantly more sensitive to  $C_{\min}$  than when  $F_{\min} = 0$ . Indeed, there is a slight local minimum in the  $TE$  versus  $C_{\min}$  behavior for the case of  $F_{\min}$  calculated according to Eq. (13). The reason for this is unclear, since this would suggest that the use of less spectral information yields improved accuracy in this case. As seen in Fig. 3, the minimum value of  $F$  calculated according to Eq. (13) can become very high as  $C_{\min}$  is

increased, leading to the artificial increase in the spectral windows and the exclusion of significant spectral absorption content.

The aforementioned unusual local minimum aside, it appears from Fig. 4 that  $T_b \approx T_{ave}$  yields the most accurate predictions, perhaps because the use of either  $T_b = T_{min}$  or  $T_b = T_{max}$  results in more extreme spectral conditions for the calculation of the ALBDF. The predictions for  $T_b = T_{ave}$  shown in Fig. 4 are very good as  $C_{min}$  approaches the value used in the generation of the ALBDF, with  $TE$  being below 5% except for the highest layer thickness. The data of Fig. 4 also suggest that while the value of  $C_{min} = 10^{-4} \text{ m}^2/\text{mol}$  used by Pearson *et al.* [7] in the generation of the ALBDF database yields very good results, even greater accuracy may be possible if the database is extended to lower values of  $C_{min}$ .

Finally, Fig. 4 seems to suggest that with the exception of the high temperature case at larger layer lengths, the prediction error’s dependence on the blackbody source temperature  $T_b$  is reduced as  $C_{min} \rightarrow 0$ , *i.e.*, as the ALBDF database becomes sufficiently deep. Indeed, for these predictions carried out with  $n = 25$  gray gases, the results show that the model predictions become independent of the value of  $T_b$  used except when  $T_b = T_{ave}$  is specified in the model spectral construction. This is an apparent contradiction of the presumption that predictions should be completely independent of the value of  $T_b$  used in the spectral construction of the model. Figure 5 explores this further, illustrating in an expanded way the dependence of the accuracy on the number of gray gases used for the most demanding case, the 800 – 2800 K temperature range with  $L = 5.0 \text{ m}$  layer length. The full possible ALBDF database,  $C_{min} = 10^{-7} \text{ m}^2/\text{mol}$ , has been used to ensure that the maximum possible spectral content is used. The figure shows total absolute error predictions for three values of the blackbody source temperature used,  $T_b = T_{min}$ ,  $T_b = T_{ave}$ , and  $T_b = T_{max}$ . It should also be noted that the abscissa has been plotted on a logarithmic scale. Figure 5 shows that whereas predictions made using  $T_b = T_{ave}$  and  $T_b = T_{max}$  achieve an unchanging accuracy for  $n \geq 6$  gray gases, the simulation using  $T_b = T_{min}$  are very sensitivity to the number of gray gases. Indeed, the total error is still decreasing for  $n = 1000$  gray gases. The conclusion is that when specifying  $T_b = T_{min}$

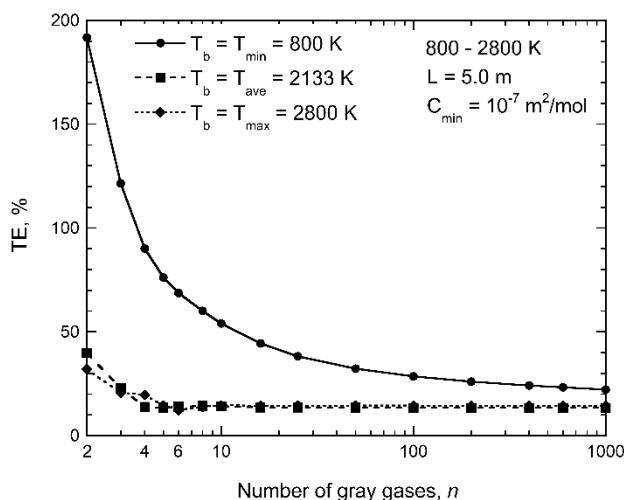


Figure 5. Dependence of the total absolute relative error on the number of gray gases used in the simulation for the 800 – 2800 K temperature range with  $L = 5.0$  m and  $C_{min} = 10^{-7}$  m<sup>2</sup>/mol.

it is much more difficult to achieve accurate numerical resolution. However, the results of Fig. 5 do confirm that *if accurately resolved numerically*, predictions using the Rank Correlated SLW model are independent of the value of the blackbody source temperature used. This is consistent with the assertions stated previously [9,10], where the value of  $T_b$  is stated to be simply a mathematical convenience in the construction of the spectral model. Vanishing dependence on  $T_b$  appears possible only in the case where *i)* the range of  $C$  in the ALBDF database is sufficiently wide, and *ii)* where sufficient numerical resolution is achieved, which appears to be accomplished most efficiently with the fewest number of gray gases when  $T_b \approx T_{ave}$  is specified.

Figure 6 shows examples of prediction of the local net radiative flux divergence  $Q$  and local absolute relative error  $LE$  using  $n = 25$  gray gases for two sample conditions using both methods of specifying  $F_{min}$  with  $C_{min} = 10^{-7}$  m<sup>2</sup>/mol. The accuracy is reasonable for engineering purposes using both methods, for these two cases. As expected, both methods for specifying  $F_{min}$  yield virtually identical results when the full ALBDF database is used (*i.e.*,  $C_{min} = 10^{-7}$  m<sup>2</sup>/mol is the lower limit of the lookup table). The local error in the lower temperature case is very good, with

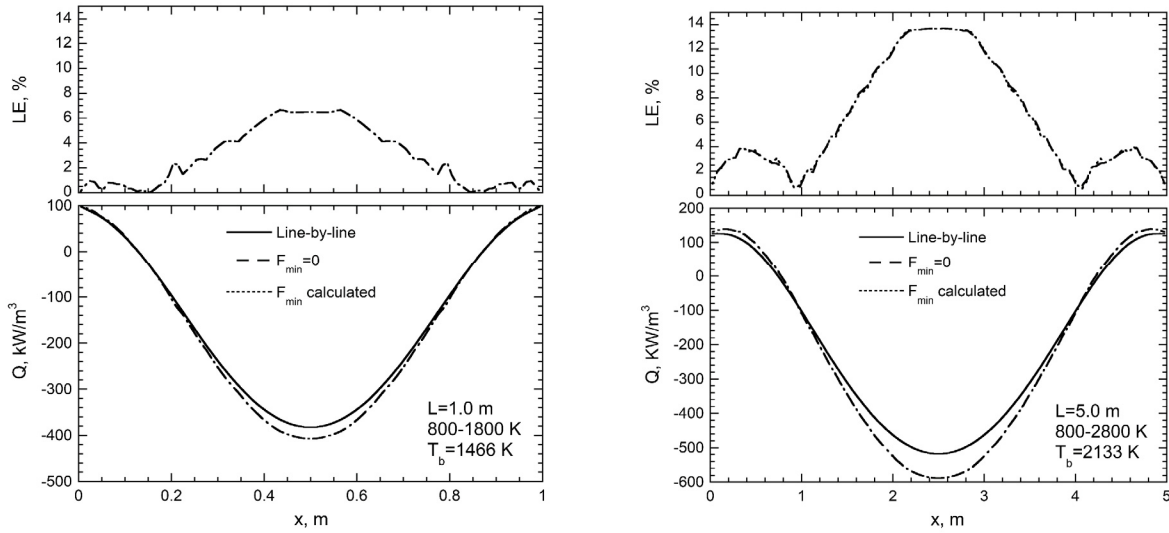


Figure 6. Predictions of local total radiative flux divergence  $Q$  and local relative absolute error  $LE$  using  $n = 25$  gray gases, for  $C_{\min} = 10^{-7} \text{ m}^2/\text{mol}$ , and  $F_{\min}$  calculated according to Eq. (13) and  $F_{\min} = 0$ :  $L = 1.0 \text{ m}$ ,  $800 - 1800 \text{ K}$ ,  $T_b = T_{\text{ave}} = 1466 \text{ K}$ ;  $L = 5.0 \text{ m}$ ,  $800 - 2800 \text{ K}$ ,  $T_b = T_{\text{ave}} = 2133 \text{ K}$ .

a maximum error of approximately 7%. It is reassuring that the prediction agreement in the extreme temperature case,  $800 - 2800 \text{ K}$ , is quite good given the significant temperature differences and corresponding extreme local gas absorption spectra that exist in the system.

Figure 7 illustrates the variation of the total absolute relative error with the number of gray gases used in the RC-SLW prediction in the range  $2 \leq n \leq 25$  for  $T_b = T_{\text{ave}}$  and for the three layer thicknesses and two temperature ranges studied. Data are shown for  $C_{\min} = 10^{-7} \text{ m}^2/\text{mol}$  with  $F_{\min}$  calculated according to Eq. (13), and for  $F_{\min} = 0$ . The gray gases are deployed according to the Gauss-Legendre quadrature node points in the range  $F_{\min} < F < F_{\max}$ . Understandably, the greater the number of gray gases used in the simulations the higher the fidelity with which the  $F$ -variable is integrated. Figure 6 shows generally that the total error is highest with  $n = 2$ , and that the error decreases to an unchanging value as the number of gray gases  $n$  increases. As expected, the total error does not vanish at large  $n$  despite the fact that the solutions approach the continuous RC-SLW solution [8]. This is because the minimum error achievable is dictated by the approximations associated with the rank correlated assumption in the RC-SLW method and the Multiplication

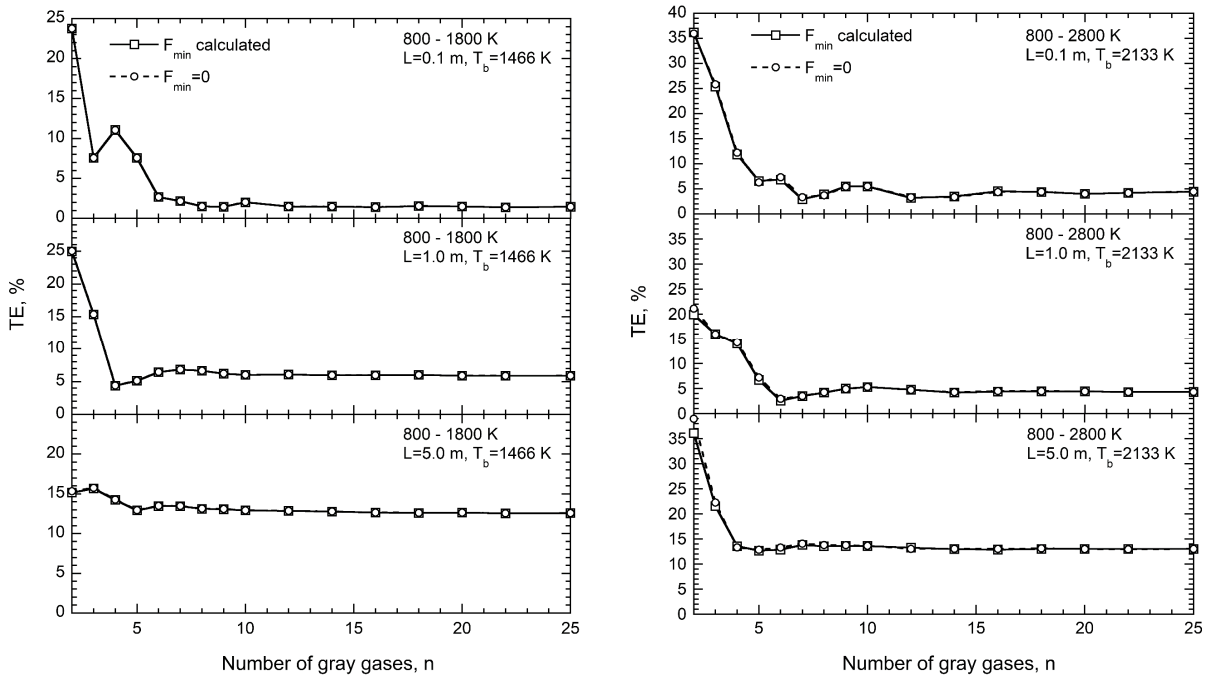


Figure 7. Dependence of the total error on the number of gray gases used in the prediction for  $T_b = T_{ave}$  for the three layer thicknesses and two temperature ranges studied, with  $C_{min} = 10^{-7}$   $m^2/mol$ .  $F_{min}$  is calculated according to Eq. (13) and  $F_{min} = 0$ .

Approach used for handling the gas mixture. Figure 6 shows that the total error’s dependence on  $n$  may not be monotonic, and oscillations are observed for some conditions for  $n < 7$ . This may be due to the complex relationship between  $F$  and  $F^{loc}$  in the RC-SLW model, with deployment of  $F$  using Gauss-Legendre quadrature node points producing higher accuracy even when fewer gray gases are used in some cases. For all cases the error ceases to change appreciably for increases in the number of gray gases above  $n \approx 10$ , suggesting that using more gray gases is unnecessary for improved accuracy. However, it can be seen that acceptable predictions are often obtained with as few as 3 - 4 gray gases.

Finally, it may be mentioned that a recent work has shown that the rank correlated spectrum assumption may be applied to the Full Spectrum correlated- $k$  (FSK) model [19]. That work revealed that the two formulations (RC-FSK and RC-SLW models) are virtually identical, and when



implemented the same way (using the same numerical solution technique and resolution, and the same spectral database) the two models yield identical results.

## CONCLUSIONS

This paper has explored the spectral model input parameters for the Rank Correlated SLW model, comparing the predictions against line-by-line benchmark predictions. The range of the ALBDF database has also been studied as it relates to accurate prediction of emissivity, and the RC-SLW model construction and prediction accuracy. Results show that model predictions are very good, and exhibit some sensitivity to the method used to specify  $F_{\min}$ . Further, although very good accuracy is demonstrated in the model it appears that improvements might be possible if the ALBDF database were extended below what was previously available. Consequently, the database has been regenerated as part of this work, extending by three decades the minimum absorption cross-section. It has been demonstrated that RC-SLW model predictions are independent of the blackbody source temperature used in the model spectral construction provided that the numerical solution has sufficient resolution. It appears that the optimal accuracy may be achieved by specifying a blackbody source temperature near the spatial average temperature in the domain. Finally, it is shown that good accuracy may be achieved using the RC-SLW model with as few as 3 – 5 gray gases, and the results are virtually insensitive to the number of gray gases used when that number is greater than  $n \approx 10$ .

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