The Development of Updated and Improved SLW Model Parameters and Its Application to Comprehensive Combustion Predictions

John T. Pearson

Brigham Young University - Provo
The Development of Updated and Improved SLW Model Parameters and Its Application to Comprehensive Combustion Predictions

John T. Pearson

A dissertation submitted to the faculty of Brigham Young University in partial fulfillment of the requirements for the degree of Doctor of Philosophy

Brent W. Webb, Chair
Vladimir P. Solovjov
Matthew R. Jones
Dale R. Tree
Thomas H. Fletcher

Department of Mechanical Engineering
Brigham Young University
October 2013

Copyright © 2013 John T. Pearson
All Rights Reserved
ABSTRACT

The Development of Updated and Improved SLW Model Parameters and Its Application to Comprehensive Combustion Predictions

John T. Pearson
Department of Mechanical Engineering, BYU
Doctor of Philosophy

Accurate modeling of radiative heat transfer through combustion gases has received considerable attention in recent years. The spectral line weighted-sum-of-gray-gases (SLW) model was developed based on detailed line-by-line spectral data of gases. A critical element of the SLW model is the absorption line blackbody distribution function (ALBDF). This function was designed to utilize the spectral properties of gases in an efficient and compact manner. However, there are several limitations of the ALBDF in its original form. First, the valid ranges of temperature and pressure are not large enough to include important applications, such as oxy-combustion, where temperatures can exceed 2500 K, and pressurized combustion, where non-atmospheric pressures are expected. In addition, since the original ALBDF correlation was developed, new spectral data have become available which extend the accuracy of the previous work. Finally, it is desirable to be able to represent the ALBDF of CO in addition to H₂O and CO₂. Improving the SLW model in this manner will make it more generally applicable and ensure greater confidence in its accuracy.

Line-by-line absorption cross-section data were generated carefully using a recently released spectroscopic database, HITEMP 2010. The Voigt line profile was implemented, and line wings were included in regions where they maintain a significant contribution. Line-by-line calculation of the ALBDF, total emissivity, and radiative transfer were also performed in order to provide benchmark data and to explore the influence of variable total pressure. It was found that increasing total pressure causes the ALBDF to shift to lower values at a given absorption cross-section, although this change is weaker at increasing temperature. Total emissivity is strongly affected by total pressure changes, although the change is modest if the product of partial pressure and pathlength is held constant. Increasing total pressure in a layer of gas increases the radiative flux exiting the gas layer; this was also found to be true for both the case of constant layer length and constant mass of radiating material.

Efficient representations of the ALBDF were generated. The hyperbolic tangent correlation of Denison and Webb was updated to reflect improved spectroscopic data and to cover a wider range of temperature (400 K ≤ T ≤ 3000 K) and pressure (0.1 atm ≤ p ≤ 50 atm). The correlation was also extended to CO, which had not been correlated previously. Using tabulated line-by-line data directly was also explored, and these data have been made available for H₂O, CO₂, and CO. Finally, these efficient representations of the ALBDF were successfully validated by comparison with line-by-line calculations and experimental data for both total emissivity and radiative transfer. The latter included comparisons with intensity measurements and a comprehensive combustion simulation implementing the SLW model.

Keywords: gas radiation, pressure, ALBDF, SLW model
ACKNOWLEDGEMENTS

This work was supported by Air Liquide. I would like to thank Jiefu Ma for his help and guidance throughout the project. Special thanks to my advisor, Professor Brent W. Webb, and also Dr. Vladimir Solovjov, for their insights, recommendations, and patience. Their expertise has been invaluable.

I would especially like to thank my wife, Kylee. Her love and support have been constant throughout my studies.
TABLE OF CONTENTS

1 Introduction ........................................................................................................................... 1

2 Review of Previous Work ..................................................................................................... 6
   2.1 Spectral Data ................................................................................................................... 6
   2.2 Global Methods ................................................................................................................ 9
   2.3 SLW Method Development .......................................................................................... 10
   2.4 SLW Modeling of Radiative Transfer .......................................................................... 13
   2.5 SLW Modeling in Multimode Heat Transfer ................................................................ 14
   2.6 SLW Method – Multi-Dimensional Scenarios ............................................................. 15
   2.7 ALBDF Development ................................................................................................... 15
   2.8 Summary ....................................................................................................................... 16

3 Detailed Line-by-Line Spectrum ....................................................................................... 17
   3.1 Accessing the Spectroscopic Database ......................................................................... 17
   3.2 Line-by-Line Formulation ............................................................................................ 19
   3.3 Mixtures of Gases ......................................................................................................... 32
   3.4 Summary ....................................................................................................................... 37

4 Total Pressure Effects on Radiative Transfer .................................................................. 38
   4.1 The Absorption Line Blackbody Distribution Function (ALBDF) .............................. 38
      4.1.1 ALBDF of Water Vapor ........................................................................................ 41
      4.1.2 ALBDF of Carbon Dioxide .................................................................................. 44
      4.1.3 ALBDF of Carbon Monoxide .............................................................................. 46
      4.1.4 Comparisons with Previous Work ........................................................................ 47
   4.2 The Planck-Mean Absorption Coefficient .................................................................. 49
   4.3 Total Emissivity at Variable Pressure .......................................................................... 51
Appendix C. Code for Efficient Calculation of the ALBDF ............................................. 145
Appendix D. SLW Code for Isothermal, Homogeneous media............................................. 158
Appendix E. Non-isothermal, Non-homogeneous SLW Code............................................ 176
Appendix F. LBL Code for 1-D Radiative Transfer .............................................................. 203
LIST OF TABLES

Table 2-1: A comparison of the number of spectral lines available in the HITEMP 2010 database and the 2008 HITRAN database ..........................................................8

Table 5-1: The correlation coefficients $b_{lmn}$ for H$_2$O (left set of H$_2$O coefficients), CO$_2$, and CO for Eq. (5-2). For H$_2$O, the coefficients $c_{lmn}$ for Eq. (5-4) are also given (right set of H$_2$O coefficients). .................................................................64

Table 5-2: The coefficients $d_{lmn}$ used in Eq. (5-5) for H$_2$O and CO$_2$ and Eq. (5-10) for CO. .......................................................................................................................69
LIST OF FIGURES

Figure 1.1: Shown are a) the absorption coefficient, $\kappa$, as a function of wavenumber, $\eta$ and b) the Planck emissive power at 1500 K normalized by the maximum emissive power, $E_{\eta}/E_{\max}$, also as a function of wavenumber. The absorption coefficient data of H$_2$O are at $T = 1500$ K, $p = 1$ atm, $Y_{H2O} = 0.01$, and for wavenumbers ranging from 0 to 10,000 cm$^{-1}$. .................................................................................................................2

Figure 3.1: The ALBDF of CO$_2$ at $T_g = T_b = 3000$ K and $p = 1$ atm. Intensity cutoff values ranging from $10^{-24}$ to $10^{-28}$ cm$^{-1}$/molecule cm$^{-2}$ are shown for comparison. ..........................................................................................................24

Figure 3.2: The number of spectral lines included in calculations for a) H$_2$O, CO$_2$, and b) CO as a function of temperature. .................................................................................................................24

Figure 3.3: The absorption cross-section, $C$, as a function of distance from line center in cm$^{-1}$ calculated using the Lorentz profile and the MT-CKD model. ............27

Figure 3.4: The spectral emissive power normalized by the maximum emissive power, $E_{\eta}/E_{\max}$, as a function of wavenumber for temperatures ranging from 500 K to 3000 K. ...............................................................................................30

Figure 3.5: Absorption cross-section as a function of wavenumber for a) H$_2$O, b) CO$_2$, and c) CO at 1500 K. The panel on the left shows the data for the full spectrum, while the panel on the right shows a small portion (3 cm$^{-1}$ wide) near 2000 cm$^{-1}$. Total pressures of 0.1, 1, 8, and 50 atm are represented. ..................................................................................................................31

Figure 3.6: The absorption cross-section, $C_{\eta}$, as a function of wavenumber, $\eta$, at a) 289 K and b) 318 K. Shown are the LBL solution generated using the present method and the experimental data from Ptashnik et al. (2013). The minimum and maximum values of the experimental data are shown, based on the margin of error for the data. .................................................................33

Figure 3.7: The ALBDF, $F$, of CO as a function of absorption cross-section, $C$, for three temperatures and three values of mole fraction of a) CO$_2$ and b) H$_2$O, as shown. For all cases, $T_g = T_b$, $p = 1$ atm, $Y_{CO} \to 0$. ..................................36

Figure 4.1: The absorption cross-section, $C$, as a function of ALBDF, $F$, is shown on the left graph. The right graph shows the corresponding spectral absorption cross-section data as a function of wavenumber, $\eta$. Gray gas $i$ is the lighter shaded region, corresponding to portions of the spectrum shown by the darker shading. ......................................................................................40
Figure 4.2: The ALBDF, \( F \), as a function of absorption cross-section, \( C \), for H\(_2\)O at a) \( T_g = T_b = 1000 \) K, and b) \( T_g = T_b = 2500 \) K for total pressures varying from 0.1 atm to 50 atm as shown. Data are shown for the limit of approaching zero mole fraction of H\(_2\)O. ..........................................................42

Figure 4.3: The ALBDF, \( F \), as a function of absorption cross-section, \( C \), for H\(_2\)O mole fractions of approaching 0 and equal to 1. The data is given at total pressures of 1 atm and 50 atm as shown. \( T_g = 1000 \) K, and \( T_b = 1000 \) K or 2500 K as shown. .......................................................................................................43

Figure 4.4: The ALBDF, \( F \), as a function of absorption cross-section, \( C \), for CO\(_2\) at a) \( T_g = T_b = 1000 \) K, and b) \( T_g = T_b = 2500 \) K for total pressures varying from 0.1 atm to 50 atm as shown. Data are shown for the limit of approaching zero mole fraction of CO\(_2\). ..................................................................................................................45

Figure 4.5: The ALBDF, \( F \), as a function of absorption cross-section, \( C \), for CO\(_2\) mole fractions of approaching zero and equal to one. The data is given at total pressures of 1 atm and 50 atm as shown. \( T_g = 1000 \) K, and \( T_b = 1000 \) K or 2500 K as shown. ...............................................................................................46

Figure 4.6: The ALBDF, \( F \), as a function of absorption cross-section, \( C \), for CO at a) \( T_g = T_b = 1000 \) K, and b) \( T_g = T_b = 2500 \) K for total pressures varying from 0.1 atm to 50 atm as shown. Data are shown for the limit of approaching zero mole fraction of CO. ..........................................................47

Figure 4.7: The ALBDF of H\(_2\)O at \( p = 1 \) atm and \( Y_{H2O} \to 0 \) for a) \( T_g = 1000 \) K and \( T_b = 500, 1500, \) and 2500 K, and b) \( T_b = 1000 \) K and \( T_g = 500, 1500, \) and 2500 K. Calculations from Denison (1994) and the ALBDF calculated using HITEMP 2010 are shown. ..........................................................48

Figure 4.8: The ALBDF of CO\(_2\) at \( p = 1 \) atm and \( Y_{CO2} \to 0 \) for a) \( T_g = 1000 \) K and \( T_b = 500, 1500, \) and 2500 K, and b) \( T_b = 1000 \) K and \( T_g = 500, 1500, \) and 2500 K. Calculations from Denison (1994) and the ALBDF calculated using HITEMP 2010 are shown. ................................................................................49

Figure 4.9: The Planck-mean absorption coefficient, \( \kappa_P \), as a function of temperature for H\(_2\)O, CO\(_2\), and CO. Shown are the line-by-line data and the calculation using the correlation based on RADCAL (Grosshandler, 1993; Barlow et al., 2001). ........................................................................................50

Figure 4.10: Total emissivity as a function of temperature for a) H\(_2\)O, b) CO\(_2\), and c) CO for \( Y_i = 0.01 \) (unless otherwise noted), \( L = 1 \) m, and total pressure as shown. Solid lines represent line-by-line predictions and dashed lines represent the Leckner correlation..........................................................52

Figure 4.11: Total net radiative flux (left graph), \( q \), and net radiative flux divergence (right graph), \(-dq/dx\), as a function of position, \( x \), for a) CO\(_2\)
and b) H$_2$O at 1000 K and $Y_i = 0.3$. Results are shown for four total pressures varying from 0.1 atm to 50 atm.

Figure 4.12: The predicted exiting total net radiative flux, $q_e$, for the three gas species investigated at a) 1000 K, and b) 2500 K.

Figure 4.13: The average relative error in the discrete ordinates solution as compared to the exact analytical solution as a function of the number of ordinate directions, $n$, for radiative flux and the divergence of the radiative flux.

Figure 4.14: The divergence of radiative flux, $-dq/dx$, as a function of position. The medium is at $p = 1$ atm, $T = 1500$ K, and $Y_{H_2O} = 0.2$. The walls are 2 m apart, and are black at 0 K.

Figure 4.15: The divergence of radiative flux, $-dq/dx$, as a function of position. The medium is at $p = 1$ atm, $T = 1300$ K, and $Y_{CO_2} = 0.3$. The walls are 5 m apart, and are at 500 K with an emissivity of 0.9.

Figure 5.1: The ratio of self- to air-broadening, $B$, as a function of temperature for H$_2$O, CO$_2$, and CO.

Figure 5.2: The ALBDF as a function of absorption cross-section for a) H$_2$O, and b) CO$_2$. The line-by-line (LBL) calculation is shown with the corresponding orthogonal polynomial correlation (OP). For the data shown, $p = 1$ atm, $Y_i \rightarrow 0$, $T_b = 1000$ K, and $T_g$ varies from 400 K to 3000 K, as shown.

Figure 5.3: The ALBDF for H$_2$O at a) $T_g = T_b = 1000$ K, and b) $T_g = T_b = 3000$ K. Shown are the line-by-line (LBL) solution, the solution taken from tabulated data, and the correlation. Total pressure is shown, and the mole fraction is $Y_{H_2O} = 0.2$.

Figure 5.4: The ALBDF for CO$_2$ at a) $T_g = T_b = 1000$ K, and b) $T_g = T_b = 3000$ K. Shown are the line-by-line (LBL) solution, the solution taken from tabulated data, and the correlation. Total pressure is shown, and the mole fraction is approaching zero.

Figure 5.5: The ALBDF for CO at a) $T_g = T_b = 1000$ K, and b) $T_g = T_b = 3000$ K. Shown are the line-by-line (LBL) solution, the solution taken from tabulated data, and the correlation. Total pressure is shown, and the mole fraction is approaching zero.

Figure 5.6: Gray gas weights, $a_j$, calculated using line-by-line data (LBL), the tabulated data, and the correlation for a) 10 gray gases, b) 25 gray gases, and c) 71 gray gases. The data were generated at $Y_{H_2O} \rightarrow 0$, $T_g = T_b = 1500$ K, and $p = 50$ atm.
Figure 5.7: Gray gas weights of H2O as a function of absorption cross-section calculated at \( Y_{H2O} \rightarrow 0 \) and a) \( T_g = T_b = 1500 \text{ K} \) and \( p = 1 \text{ atm} \), b) \( T_g = T_b = 1500 \text{ K} \) and \( p = 50 \text{ atm} \), c) \( T_g = T_b = 3000 \text{ K} \) and \( p = 1 \text{ atm} \), and d) \( T_g = T_b = 3000 \text{ K} \) and \( p = 50 \text{ atm} \) .......................................................... 85

Figure 5.8: Gray gas weights of CO2 as a function of absorption cross-section calculated at \( Y_{CO2} \rightarrow 0 \) and a) \( T_g = T_b = 1500 \text{ K} \) and \( p = 1 \text{ atm} \), b) \( T_g = T_b = 1500 \text{ K} \) and \( p = 50 \text{ atm} \), c) \( T_g = T_b = 3000 \text{ K} \) and \( p = 1 \text{ atm} \), and d) \( T_g = T_b = 3000 \text{ K} \) and \( p = 50 \text{ atm} \) ............................................................................ 86

Figure 5.9: Gray gas weights of CO as a function of absorption cross-section calculated at \( Y_{CO} \rightarrow 0 \) and a) \( T_g = T_b = 1500 \text{ K} \) and \( p = 1 \text{ atm} \), b) \( T_g = T_b = 1500 \text{ K} \) and \( p = 50 \text{ atm} \), c) \( T_g = T_b = 3000 \text{ K} \) and \( p = 1 \text{ atm} \), and d) \( T_g = T_b = 3000 \text{ K} \) and \( p = 50 \text{ atm} \) ............................................................................ 88

Figure 5.10: The computation time of a representation of the ALBDF as a function of number of calculations, \( N \). Shown are times for the hyperbolic tangent correlation for both the atmospheric correlation and for variable pressure, the time to access the tabulated data for the species investigated, and the orthogonal polynomials of order 3 and 10 .................................................. 90

Figure 6.1: Total emissivity, \( \varepsilon \), as a function of temperature and total pressure for a) H2O, b) CO2, and c) CO. Shown are line-by-line data, the solution obtained using tabulated data, and the solution obtained using the correlation. For the data shown, \( Y_i = 0.01 \) unless otherwise indicated ....................... 94

Figure 6.2: Total emissivity of H2O at \( p = 0.1, 1, \) and 2 \( \text{ atm} \) and \( p_iL = 1 \) and 100 \( \text{ cm-atm} \) as a function of temperature. Shown are data taken from Ludwig et al. (1973), calculated emissivity using line-by-line data, and emissivity generated from tabulated ALBDF data, and the ALBDF correlation ................................................................. 95

Figure 6.3: Divergence of radiative flux in a layer of H2O at a) \( T = 1250 \text{ K} \), and b) \( T = 2750 \text{ K} \). Shown are the line-by-line (LBL) solution and the solution obtained using tabulated ALBDF data or using the correlation. Total pressures of 0.1 \( \text{ atm} \), 1 \( \text{ atm} \), and 50 \( \text{ atm} \) are shown ................................................................. 98

Figure 6.4: Divergence of radiative flux in a layer of CO2 at a) \( T = 1250 \text{ K} \), and b) \( T = 2750 \text{ K} \). Shown are the line-by-line (LBL) solution and the solution obtained using tabulated ALBDF data or using the correlation. Total pressures of 0.1 \( \text{ atm} \), 1 \( \text{ atm} \), and 50 \( \text{ atm} \) are shown ................................................................. 99

Figure 6.5: Divergence of radiative flux in a layer of CO at a) \( T = 1250 \text{ K} \), and b) \( T = 2750 \text{ K} \). Shown are the line-by-line (LBL) solution and the solution obtained using tabulated ALBDF data or using the correlation. Total pressures of 0.1 \( \text{ atm} \), 1 \( \text{ atm} \), and 50 \( \text{ atm} \) are shown ................................................................. 100
Figure 6.6: Divergence of radiative flux at 0.1, 1, and 50 atm in a gas mixture exhibiting a stepwise temperature and concentration profile for a) 1000 K and 1500 K, and b) 2000 K and 3000 K. Shown are the line-by-line (LBL) solution, the solution obtained using the tabulated data, and the solution obtained using the correlation.

Figure 6.7: The experimental temperature measurements taken from the BERL reactor for a) the cold wall cases, and b) the hot wall cases. The solid lines represent data measured at AD/D_0 = 0.31 and the dashed lines represent measurements taken at AD/D_0 = 1.25.

Figure 6.8: The experimental mole fraction measurements for H_2O, CO_2, and CO taken in the BERL reactor for a) the cold wall cases, and b) the hot wall cases. The solid lines represent data measured at AD/D_0 = 0.31 and the dashed lines represent measurements taken at AD/D_0 = 1.25.

Figure 6.9: Comparison of experimental radiative intensity measurements and SLW predictions as a function of distance from the furnace wall for a) AD/D_0 = 0.31 and b) AD/D_0 = 1.25. Shown are data for the case of both cold walls (T_w = 300 K) and hot walls (T_w = 758 K), as indicated.

Figure 6.10: The propane burner used by Andersson et al. (2008).

Figure 6.11: The mesh used in FLUENT simulations. Shown on the mesh are the burner region (red), the furnace exit (blue), and at 384 mm and 1400 mm, the locations where experimental data were reported (green lines).

Figure 6.12: The temperature field in degrees C resulting from the FLUENT simulation when the WSGG model was implemented.

Figure 6.13: Shown are the resulting temperature distributions of the FLUENT simulation in degrees C in which the SLW method was used incorporating a) the tabulated data, and b) the correlation.

Figure 6.14: Shown are the temperature distributions at a) 384 mm, and b) 1400 mm downstream from the burner. Data are given for the experimental measurements and for each of the three FLUENT simulations.

Figure 6.15: Shown are the H_2O mole fraction distributions at a) 384 mm, and b) 1400 mm downstream from the burner. Data are given for the experimental measurements and for each of the three FLUENT simulations.

Figure 6.16: Shown are the CO_2 mole fraction distributions at a) 384 mm, and b) 1400 mm downstream from the burner. Data are given for the experimental measurements and for each of the three FLUENT simulations.
Figure 6.17: The radiative intensity measured at a) 384 mm and b) 1400 mm from the burner. Shown are experimental measurements and SLW predictions implementing the tabulated data and correlation. ........................................116

Figure 6.18: The divergence of radiative flux, $-dq/dx$, as a function of position a) in the flame region (384 mm), and b) downstream of the flame (1400 mm). Data are given for the FLUENT simulations implementing the SLW method and for one-dimensional SLW predictions, both of which are implemented using both the tabulated data and the correlation.........................117
1 INTRODUCTION

Modeling radiative heat transfer in high-temperature gases in an accurate and efficient manner is a difficult problem that has received considerable attention in recent years. The efficiency of any approach to modeling radiative transfer in such situations is particularly important in comprehensive combustion simulations, where prediction of the radiative transfer is perhaps the most computationally intensive part of the overall simulation. The major complication when dealing with radiation transfer in gases is that the absorption coefficient has a strong spectral dependency. The spectral absorption coefficient is characterized by vibration-rotation bands in which thousands of absorption lines are grouped. The absorption coefficient can vary by several orders of magnitude over a relatively short spectral range. This is illustrated in Figure 1.1 where the spectral absorption coefficient, $\kappa_\eta$, is plotted as a function of wavenumber, $\eta$. The data shown are for a small concentration of H$_2$O (mole fraction $Y_{H_2O} = 0.01$) at a temperature of 1500 K and total pressure of 1 atm. Shown for comparison is the Planck emissive power as a function of wavenumber normalized by the maximum emissive power for this scenario. For H$_2$O at these conditions, there are about 1.7 million spectral lines that have a significant contribution to the absorption coefficient calculation.

There are a number of modeling approaches that are designed to capture these significant spectral variations. The rigorous line-by-line approach fully accounts for spectral variations by integrating over wavenumber. This is done by integrating the Radiative Transfer Equation within
Figure 1.1: Shown are a) the absorption coefficient, $\kappa$, as a function of wavenumber, $\eta$, and b) the Planck blackbody emissive power at 1500 K normalized by the maximum emissive power, $E_\eta/E_{\text{max}}$, also as a function of wavenumber. The absorption coefficient data of H$_2$O are at $T = 1500$ K, $p = 1$ atm, $Y_{\text{H}_2\text{O}} = 0.01$, and for wavenumbers ranging from 0 to 10,000 cm$^{-1}$.
wavenumber intervals small enough to capture the data exactly and then summing the result. However, due to the extensive spectral data that are used in these calculations, this method is not computationally practical in realistic engineering situations. At the other extreme, the gray approach removes spectral dependency of the absorption coefficient altogether by selection of an average value for all wavenumbers. This approach requires the least computation time, but is known to lead to significant and unacceptable error.

There are several methods that fall between these two extremes, and seek to achieve the accuracy of line-by-line calculations with efficiency close to that of the gray model assumption. Narrow band models comprise one such family of solution methods that propose using relatively narrow wavenumber intervals where an average value of the absorption coefficient can be used. Wide band models integrate over larger wavenumber intervals utilizing the fact that blackbody intensities do not vary substantially across bands. Wide band models are less computationally expensive than narrow band models but do not achieve the same level of accuracy (Modest, 2003).

Global models alter the integration scheme by integrating over absorption coefficient instead of wavenumber, and by using this engineering approach near-line-by-line accuracy is possible using significantly less computational resources than the line-by-line approach. Whereas a line-by-line calculation may require integration of the radiative transfer equation (RTE) millions of times for prediction of total (spectrally integrated) quantities such as radiative flux and net flux divergence, global models typically require fewer than 20 integrations.

One popular global model is the spectral line weighted-sum-of-gray-gases (SLW) model (Denison and Webb, 1993a). This model was initially developed in the 1990’s, and a number of improvements and extensions of the model have been reported since its initial development. The
technical development of the SLW model will be described in detail in Chapter 2. A central element of the SLW model is the absorption line blackbody distribution function (ALBDF). The ALBDF is a mathematical expression that utilizes the spectral properties of gases in order to yield model parameters in a compact form and can be calculated rigorously using line-by-line data. The ALBDF was originally represented using a hyperbolic tangent function (Denison and Webb, 1993b). Recently, an updated and improved spectral database, HITEMP 2010 (Rothman, 2010) has been published that improves the accuracy of spectroscopic data, with the possibility of updating the previous correlation of the ALBDF in its original form (Denison and Webb, 1993b). The new data also make it more reasonable to accurately extend the ALBDF to higher temperatures. The initial ALBDF correlation was recommended for the temperature range 400 K to 2500 K, whereas some oxycombustion applications can experience temperatures as high as 3000 K. Further, most spectral calculations are done at atmospheric pressure, while some combustion applications such as gas turbines and gasifiers are designed to operate at significantly higher total pressures. The effects of variable total pressure on the ALBDF have not been adequately addressed previously. Finally, the ALBDF was originally correlated for H₂O and CO₂, but a correlation for CO has not been published. While this species generally has a weaker contribution to radiative transfer in most engineering applications, its impact cannot be neglected for some situations.

The objective of the present research is to address the shortcomings mentioned above. New spectral absorption data will be generated based on the updated HITEMP 2010 database, and the ALBDF will be generated based on the updated spectroscopic information. Further, correlations of the ALBDF for H₂O and CO₂ will be revised based on the new spectral database. The ALBDF will be expanded to a larger temperature range. No correlation for the ALBDF of
carbon monoxide exists at present, so this correlation will be generated. Finally, the effects of variable total pressure on radiative transfer in these three gas species will be carefully characterized, and the representations of the ALBDF will be expanded to account for variable total pressure. The existing form of the empirical correlation of the ALBDF has been the focus of the study, but other forms have also been investigated and that will be summarized here. Because of the expanded computational capabilities now available, one of these alternative approaches to representing the ALBDF will be to use tabulated line-by-line data directly.

As mentioned, Chapter 2 will describe the previous technical development of the SLW model. In addition, other pertinent literature will be reviewed. Chapter 3 will provide a detailed description of the line-by-line generation of data using the HITEMP 2010 spectroscopic database. A description of how to access the HITEMP 2010 database will be given. This will be followed by the line-by-line development for calculating the absorption cross-section as a function of wavenumber. Obtaining line-by-line calculations of the ALBDF and other quantities of interest will be presented in Chapter 4. This description will be accompanied by an illustration of the effects of total pressure on both the ALBDF and predicted radiative transfer in high-pressure environments. Chapter 5 will describe the correlation of the ALBDF, accessing the ALBDF using tabulated data, and address issues regarding these representations of the ALBDF. The correlated and tabulated ALBDF will be validated in Chapter 6 primarily using the line-by-line solution as benchmark, but also with experimental data where such data exist. Chapter 7 will give conclusions and suggestions for future development. Many of the computer codes used as part of this study, written in C++, are included in the appendices.
2 REVIEW OF PREVIOUS WORK

When modeling radiation influences in participating media, the Radiative Transfer Equation (RTE), must be solved. This equation governs the transport of radiant energy. The one-dimensional non-scattering spectral form of the RTE is given as

$$\frac{dI_\eta(s,\Omega)}{ds} = -\kappa_\eta(s)I_\eta(s,\Omega) + \kappa_\eta(s)I_{b\eta}[T(s)], \quad (2-1)$$

where $I_\eta$ is the spectral intensity at wavenumber $\eta$, $\kappa_\eta$ is the spectral absorption coefficient, $I_{b\eta}$ is the blackbody intensity at local temperature $T(s)$, and $s$ is the position. The spectral intensity is a function of both angular direction $\Omega$ and spatial position $s$.

The standard approach to accounting for the spectral dependence of the RTE is to integrate over wavenumber to determine the total intensity, from which the local radiative flux and local radiative flux divergence may be evaluated. The local radiative flux divergence then appears as the source term in the governing equation of energy transport. Integration of the RTE over wavenumber is a computationally intensive endeavor in radiatively participating gases, as will be described below.

2.1 Spectral Data

For radiatively participating gases such as H$_2$O, CO$_2$, and CO, the absorption coefficient, $\kappa_\eta$, exhibits thousands of spectrally narrow lines grouped in vibration-rotation bands. In order to
calculate radiative transfer in gases, spectral data must be applied correctly. Spectroscopic databases have been assembled that provide detailed parameters for absorbing and emitting lines for a number of important species. HITRAN (high-resolution transmission molecular absorption database) is a database initially released in 1973 (McClatchey et al., 1973) for documenting the spectroscopic behavior of gases at or near room temperature, and the database has since been periodically expanded and revised. The most recent version was released in 2008 (Rothman et al., 2009). The 1996 version of HITRAN was released with software, called JavaHAWKS, which is an interface tool to allow easy access to the database (Rothman et al., 1998). However, JavaHAWKS has since become somewhat dated, and the availability of a replacement interface tool is expected (Rothman et al., 2009). As mentioned, the HITRAN database is intended for low to moderate temperatures, such as what is typical for atmospheric conditions. Thus it is expected to have limited applicability to combustion applications.

The HITEMP database (high-temperature molecular database) is similar to HITRAN, but is intended for higher temperature use. The first version of HITEMP was released in 1995 (Rothman et al., 1995). The 1995 HITEMP database was intended to be valid up to temperatures of 1000 K, and an extension up to 1500 K for H$_2$O was released later. More recently, a new version of HITEMP was released which is intended for temperatures up to 4000 K (Rothman et al., 2010). This version, the HITEMP 2010 database, has not been broadly used to date but provides a significant expansion over the HITRAN database. Table 2-1 shows a comparison of the number of spectral lines available in the two databases, 2008 HITRAN and HITEMP 2010 (Rothman et al., 2010). As can be seen, the HITEMP 2010 database contains significantly more spectral lines than HITRAN. The reason for this is that as temperatures increases, the spectral
lines typically increase in significance, and therefore more lines are required for accurate calculations at high temperature.

Table 2-1: A comparison of the number of spectral lines available in the HITEMP 2010 database and the 2008 HITRAN database.

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Number of Spectral Lines HITEMP 2010</th>
<th>Number of Spectral Lines 2008 HITRAN</th>
</tr>
</thead>
<tbody>
<tr>
<td>H$_2$O</td>
<td>111,377,777</td>
<td>69,201</td>
</tr>
<tr>
<td>CO$_2$</td>
<td>11,167,618</td>
<td>312,479</td>
</tr>
<tr>
<td>CO</td>
<td>115,218</td>
<td>4,477</td>
</tr>
</tbody>
</table>

Another prominent spectral database is the CDSD-1000 database, which documents spectroscopic line information for CO$_2$ (Tashkun et al., 2003). The HITEMP 2010 database incorporated the CDSD-1000 database, in expanded and enhanced form (Rothman et al., 2010). CDSD-4000 gives line information for CO$_2$ that is intended for the temperature range 2500 K up to 5000 K (Tashkun and Perevalov, 2011). A recent study showed that using the HITEMP 2010 database leads to a significant difference in radiation calculations compared to other databases, with differences up to 50% (Chu et al., 2011).

In applying the spectral data in one of these databases, an absorption line shape must be appropriately selected. The Lorentz line profile describes the absorption cross-section distribution of a line that is broadened by collisions (Modest, 2003), and has been used extensively, including in the development of the previous correlations of the absorption line blackbody distribution function (ALBDF) for H$_2$O and CO$_2$ (Denison and Webb, 1993b; Denison and Webb, 1995a). The Voigt line profile is a convolution of the Lorentz and Doppler
line profiles. The Voigt profile is more accurate for cases of low pressure and/or high temperature (Modest, 2003; Wang and Modest, 2004). Further, it has been well established that the Lorentz line profile, which is the dominant element of the Voigt line profile for the conditions explored in this study, over-predicts the absorption cross-section in the far-wing regions of the line (Mlawer et al., 2012; Perrin and Hartmann, 1989). These studies propose a correction factor, $\chi$, to adjust the line shape to match available experimental data more closely for H$_2$O (the MT-CKD model) and for CO$_2$. However, the MT-CKD model is only intended for applications near room temperature and atmospheric pressure (Mlawer et al., 2012). A recent paper suggests that the MT-CKD model significantly under-predicts the spectral absorption cross-section, $C_\eta(p,T,Y_i)$, in the spectral window regions between vibration-rotation bands (Ptashnik et al., 2013). The $\chi$ factor for CO$_2$ has been reported to be applicable to temperatures as high as 800 K and for pressures ranging from 0 to 60 bars (Perrin and Hartmann, 1989).

### 2.2 Global Methods

The detailed nature of the spectral data renders line-by-line (LBL) integration prohibitively expensive. Recently, global methods have been developed that propose integration over the absorption coefficient rather than wavenumber. These methods will now be briefly summarized.

The SLW method was perhaps the first global method to propose integration over absorption cross-section (or absorption coefficient) in engineering applications (Denison and Webb, 1993a). The absorption line blackbody distribution function (ALBDF) was conceived as part of this method development, and the function was generated for H$_2$O (Denison and Webb, 1993b) and CO$_2$ (Denison and Webb, 1995a). The SLW method will be presented in greater detail in sections to follow.
The full-spectrum \( k \)-distribution (FSK) method is also a promising global model, and was first introduced by Modest and Zhang (Modest and Zhang, 2000; Zhang, 2002). The FSK method proposes solution of the RTE by integration over a distribution function virtually identical to the ALBDF of Denison and Webb (1993b). The method is mathematically complex, but yields excellent accuracy, producing exact predictions for isothermal, homogeneous systems if integrated appropriately. Since its introduction, the FSK model has undergone further refinement, expanded for use with gas-particulate mixtures (Modest and Zhang, 2002), multi-dimensional media (Mazumder and Modest, 2002), non-homogeneous gas mixtures (Zhang and Modest, 2002; Wang and Modest, 2005a; Pal et al., 2008), and non-homogeneous gas mixtures with soot (Pal and Modest, 2010). The FSK method has been shown to be equivalent to a form of the SLW method when the number of gray gases tends to infinity (Solovjov and Webb, 2009), thus illustrating the relationship between the two models.

Another prominent global model is the absorption distribution function (ADF) model. It was first introduced by Rivière et al. (1996). The ADF model is almost identical to the SLW model (Modest and Zhang, 2002; Pierrot et al., 1999a) and only differs in implementation. The absorption distribution function model with fictitious gases (ADFFG) was developed to extend the ADF method to the treatment of non-isothermal media (Pierrot et al., 1999a). It has been shown that, for the case of non-isothermal media, the ADF and SLW models yield comparable accuracy, while the ADFFG model gives more accurate results than the SLW or ADF models at the expense of computation time (Pierrot et al., 1999b).

2.3 SLW Method Development

As mentioned previously, the first global model to be published is the SLW model, presented by Denison and Webb (1993a). It has been shown that in the limiting case as the
number of gray gases tends to infinity the SLW model is exact for isothermal, uniform media. Further, the method can be used with non-black boundaries.

Denison and Webb introduced the ALBDF as an integral part of and simultaneous to the SLW model (Denison and Webb, 1993b). For a gas at known temperature, the ALBDF is a representation of the fraction of the blackbody energy in all wavenumber regions for which the spectral absorption cross-section is below a prescribed value. This is illustrated in detail in Section 4.1. Empirical correlations for the ALBDF for H₂O were developed in the form of a hyperbolic tangent function (Denison and Webb, 1993b), a form that has been widely used since its introduction. Correlations for CO₂ were subsequently reported (Denison and Webb, 1995a), also using the hyperbolic tangent form of the correlation. These correlations were originally developed using a least-squares fit to ALBDF data generated using detailed line-by-line (LBL) data from the HITRAN database supplemented with hot lines (spectral lines that are significant only at elevated temperatures) generated using approximate spectroscopic theory. Use of the ALBDF correlation combined with the SLW model was soon thereafter introduced (Denison and Webb, 1994). Model parameters for carbon monoxide have also been proposed (Solovjov and Webb, 1998), and it has been shown that the influence of CO on radiative transfer should be taken into account for certain conditions (Solovjov and Webb, 2006). The ALBDF is also used in the other global models, and is called the cumulative $k$-distribution (FSK model) and the absorption distribution function (ADF model), but the distribution function is identical.

When non-isothermal or non-homogeneous media is considered, spectral integration of the RTE leads to the appearance of additional terms as a result of the Liebnitz rule of integration (Denison, 1994). These terms have been treated in the SLW model using two approaches. The first, called the reference approach, allows the Liebnitz terms to cancel through use of a
reference state. Perhaps the main difficulty using this method is that a set of parameters must be calculated implicitly, a process which can be computationally expensive. The second approach is to simply neglect the Liebnitz terms in the RTE (Solovjov and Webb, 2000), although this can lead to significant error in some cases and is typically less accurate than the reference approach.

A number of approaches for treating radiative transfer in mixtures of gases in the context of the SLW method have also been proposed. The double-integration method and convolution methods were initially introduced only for mixtures of H$_2$O and CO$_2$ (Denison and Webb, 1995c), and were later generalized to an arbitrary number of species (Solovjov and Webb, 2000). The superposition and multiplication approaches, along with a hybrid of the two, were also introduced (Solovjov and Webb, 2000). Including soot as a “gas” in the multiplication method has been successfully implemented as well (Solovjov and Webb, 2001).

In addition to the practical challenges of modeling radiation transfer in non-isothermal, non-homogeneous gases and gas mixtures, there are often engineering applications where the total pressure in the system of interest differs from atmospheric pressure. Extending the empirical correlations for the ALBDF to high pressure is thus of interest. Denison and Webb proposed correlations that extend the ALBDF to high pressure (Denison and Webb, 1996a), although this work was preliminary, did not appear in the archival literature, and has not been widely adopted. Providing updated and generally acceptable representations of the ALBDF for elevated pressure is one of the objectives of this work.

Other modifications and extensions to the SLW method have been proposed. Recently, the SLW model has been used in combination with the cumulative wavenumber (CW) method using a multi-layer approach (Solovjov and Webb, 2008). This method has been shown to be very accurate. Further, the SLW-1 model has been developed (Solovjov et al., 2011), which
proposes implementation of the SLW method with only one gray gas and one clear gas, whose properties are optimized. This method retains much of the accuracy of the original SLW model at significant savings in computational cost.

Another recent paper details the exact limit of the SLW model (Solovjov and Webb, 2009). In the limit of an infinite number of gray gases in the SLW model, two exact forms of the SLW model result, one of which is shown to be equivalent to the FSK method, as has been mentioned. This has shown that in their fundamental form (prior to implementation of an integration scheme) the SLW and FSK methods are virtually identical.

Detailed reviews of the SLW model have been given (Denison and Webb, 1996b; Webb, 1999). Also, the Ph.D. dissertations of Denison (1994) and Solovjov (1999) give detailed descriptions of its development.

2.4 SLW Modeling of Radiative Transfer

The SLW model has been used extensively to model radiation heat transfer in high temperature gases. The SLW method has been successfully implemented to model radiation interactions in a simulation of an industrial flame (Lallemant et al., 1996). Use of the SLW approach in conjunction with the method of lines has been shown to yield excellent predictions when modeling radiation (Cayan and Selçuk, 2007). Radiative intensity in an oxy-fuel boiler has been successfully modeled using the SLW model, and experimental data for this case have validated the study (Johansson et al., 2010). A number of different radiation models, including the gray model, the statistical narrow band model, the FSK model, and the wide band model have been compared to the SLW model for a non-gray sooting media (Demarco et al., 2011). The study showed that the SLW and FSK models were the best choices for a compromise with accuracy and computation time.
Very few studies that implement the SLW model at non-atmospheric pressure conditions have been reported. One such study that was performed utilized the SLW model in a rocket nozzle where strong pressure gradients were present (Badinand and Fransson, 2002). In this study, the reference approach was implemented in order to treat thermodynamic property gradients (including total pressure) and it was found that the results exhibited a modest dependence on the choice of reference pressure.

2.5 SLW Modeling in Multimode Heat Transfer

The SLW model has also been used in more comprehensive studies that involved combinations of heat transfer modes. It was successfully implemented in conjunction with a turbulent reacting flow model for prediction of the structure of a non-luminous turbulent jet diffusion flame (Coelho et al., 2003). The SLW model was used to predict interactions in an aluminum recycling furnace, modeling the radiative effect of a thin layer of dross on the surface on heat transfer to the molten aluminum (Solovjov and Webb, 2005). It has also been applied to combustion of biomass in a combustion chamber with adiabatic walls (Klason et al., 2008). This study compared experimental data collected to the numerical predictions, showing reasonable agreement. The SLW model in combination with a natural convection model in a thermal cavity has been studied (Colomer et al., 2007). This study concluded that using fewer optimized gray gases is the preferred approach, since it reduces the number of operations while still yielding accurate results. Another study that coupled radiation and convection in a cavity revealed that radiation has a strong influence on temperature and concentration fields (Meftah et al., 2009). The SLW model was compared to predictions from several other radiation models in pool fire simulations, and for this case all radiation models tested showed reasonable agreement (Krishnamoorthy, 2010).
2.6 SLW Method – Multi-Dimensional Scenarios

A few studies have focused on use of the SLW model for multi-dimensional radiative transfer simulations. When modeling radiation in a two-dimensional enclosure (Goutiere, 2000) or a three-dimensional enclosure (Coelho, 2002), the SLW model stood out among other models as a good compromise between accuracy and computation time. Another study combined the SLW method with the method of lines, implemented in a three-dimensional enclosure, and reported accurate solutions (Selçuk and Doner, 2009). A comparison of the SLW model with the cumulative wavenumber (CW) method and two simpler models (WSGG and gray model) in a two-dimensional axisymmetric diffusion flame showed that the SLW and CW methods both yield good results for the radiation source term but have a higher computation time than the other models tested (Mossi et al., 2010).

2.7 ALBDF Development

Of particular interest is the ALBDF, since the correlations of Denison and Webb (Denison and Webb, 1993b; Denison and Webb, 1995a) contain empirical coefficients based on the data that were available at the time of its publication. The ALBDF of Denison and Webb for H₂O and CO₂ were based on the 1992 HITRAN database (Rothman et al., 1992), supplemented with hot lines generated using approximate spectroscopic theory.

Since the initial release of the correlations for H₂O and CO₂, there have been attempts by other research groups to update or improve the ALBDF. Modest et al. provided updated correlations in the hyperbolic tangent form for both CO₂ using the CDSD-1000 database (Modest and Mehta, 2004), and for H₂O using the 1995 HITEMP database (Modest and Singh, 2005). Wang and Modest also described use of the ALBDF in the form of a look-up table for both H₂O and CO₂ (Wang and Modest, 2005b). More recently, Węcel et al. (2010) proposed a partial
orthogonal decomposition to represent the ALBDF. The latter two methods of representing the ALBDF are based on the 1995 HITEMP database. Also, André and Vaillon (2009) used $k$-moments to produce a database for the ALBDF of CO$_2$. This effort was based on the CDSD-1000 database. Each of these updates to the ALBDF has acceptable accuracy for use in engineering calculations, based on the spectroscopic database used. However, newer spectral data has extended the accuracy of previous databases. Further, many applications require improvements to the existing ALBDF representations, such as an extension to higher temperatures, rigorous extension to variable total pressure, the development of the ALBDF for CO, and/or higher accuracy. Providing these improvements is another objective of this work.

2.8 Summary

To summarize, the SLW method has been well developed for predicting radiative intensity (and consequently radiative flux and divergence) for cases that are homogeneous or non-homogeneous, isothermal or non-isothermal, and for mixtures of multiple gases. Special cases, such as the exact limit as the number of gray gases tends to infinity or the case of one gray gas and one clear gas, have also been successfully explored to fundamentally characterize the method. However, the ALBDF, which is an essential element of the SLW method, is based on spectral data which has been superseded by more recent and more accurate spectral data, and requires extension to variable pressure, higher temperature, and more species (CO). Robust validation of the SLW method with an updated ALBDF is an area where further research is needed.
3 DETAILED LINE-BY-LINE SPECTRUM

The generation of line-by-line (LBL) absorption spectra for the three gases of interest, H$_2$O, CO$_2$, and CO, will now be described. The principle parameter generated is the spectral absorption cross-section, $C_\eta$, which is needed for obtaining benchmark calculations for the absorption line blackbody distribution function (ALBDF), total emissivity, the Planck mean absorption coefficient, and solutions for radiative transfer. The generation of these secondary solutions will be described in the next chapter. In particular, the ALBDF benchmark data are essential in exploring efficient representations of the ALBDF. Some of the details in this chapter and in Chapter 4 appear in Pearson et al. (2013b).

3.1 Accessing the Spectroscopic Database

As mentioned in the introduction, the HITEMP 2010 database has been reported to be accurate for temperatures up to 4000 K (Rothman et al., 2010). This database contains molecular spectroscopic data for several gas species, including the three considered in this study, H$_2$O, CO$_2$, and CO. The structure of the database is similar to previous databases; however, the HITEMP 2010 database contains significantly more spectral lines and therefore, the data are separated into multiple files for H$_2$O and CO$_2$, each of which gives data for a certain spectral range. The data file for CO is small enough to be given in a single file. The files contain data for a list of spectral lines, each of which represents a discrete spectral location where the gas absorbs
or emits electromagnetic radiant energy. The database gives the isotopologue, the vacuum wavenumber, the intensity, the air- and self-broadened halfwidths, and several other quantities needed for spectral calculations. The database contains data primarily for the principle isotopologue (a molecule composed of certain isotopes) of H₂O, the 626 isotopologue (a molecule containing the oxygen-16, carbon-12, and oxygen-16 isotopes), though there are limited data for some of the other isotopologues of H₂O. Four major isotopologues of CO₂ are represented in detail. The intensities for lines of a given isotopologue are scaled by their terrestrial abundance (Rothman et al., 2010) and therefore all isotopologues can be used together for calculations, even though the principal isotopologue for each species has a natural abundance near 99%.

The HITEMP 2010 database is downloaded according to instructions found at the website http://www.cfa.harvard.edu/hitran/HITEMP.html. A software application, JavaHAWKS, was released with the 1996 version of HITRAN that interfaces with the database files to compile significant spectral lines and scale them according to temperature (Rothman et al., 1998). However, in early attempts to access the database it was discovered that the software package imposes an intensity cutoff, to be described later, prior to calculating the line intensity according to temperature. Because the spectral lines typically increase in strength as temperature increases, many lines that are only significant at high temperature are lost in this process. Further, the software is quite dated, does not allow for the computational flexibility that is required, and only performs the first of several steps that are needed to calculate the absorption cross-section. Therefore, as part of this investigation a computer code was written in C++ that performs all of the steps needed to access the line parameters in the database and compute the spectral
absorption cross-section data. The code is included in Appendix A. The detailed formulation for
the process that was followed to carry out this calculation is described in the next section.

### 3.2 Line-by-Line Formulation

Once the database is obtained the line-by-line (LBL) spectral absorption cross-section,
\( C_\eta(p,T,Y_i) \), can be generated as a function of wavenumber, \( \eta \). This quantity also exhibits a
dependence on total pressure, \( p \), gas temperature, \( T \), and the mole fraction of the species \( i \) of
interest, \( Y_i \). The following development describes the generation of the spectral absorption cross-
section for a single gas mixed with air. Air does not participate in radiative transfer. Section 3.3
describes the method used to obtain the absorption cross-section data for mixtures of
participating gases.

The Lorentz line profile is used where collision broadening is the dominant broadening
mechanism, while the Doppler line profile is employed at conditions where Doppler broadening
is dominant (Modest, 2003). The Voigt line profile is the convolution of the Lorentz and Doppler
profiles and gives more accurate results at sub-atmospheric pressure and at high temperatures
where both collision (Lorentz) and Doppler broadening can be significant (Wang and Modest,
2004; Modest, 2003). Because sub-atmospheric pressures and high temperatures are included in
this study, the Voigt profile is used. The shape for a single spectral line according to the Voigt
profile is represented by (Modest, 2003)

\[
C_{\eta,j}(p,T,Y_i) = \frac{S_j(p,T)}{\pi^{3/2}} \int_{-\infty}^{\infty} \frac{e^{-x^2}dx}{\left[ \eta - \eta_{0,j}(p) - \frac{x\gamma_{D,j}(p,T)}{\sqrt{\ln 2}} \right]^2 + \gamma_{L,j}^2(p,T)}
\]

(3-1)

where \( x = v\sqrt{M_i/2kT} \). The line intensity, \( S_j(p,T) \), the wavenumber at vacuum conditions
corresponding to the line location, \( \eta_0(p) \), and the line half-widths at half-maximum due to
Lorentz broadening, $\gamma_L(p,T)$, and Doppler broadening, $\gamma_D(p,T)$, are calculated as described subsequently. $T$ is the gas temperature, $M_i$ is the mass of the molecule of interest, and $v$ is the relative velocity of the molecule. In practice, the Humlíček algorithm (Humlíček, 1982) was used to evaluate Eq. (3-1), as no closed-form solution to the integral exists.

The Lorentz and the Voigt profiles were compared using calculations of the ALBDF. The ALBDF was used as the basis for this and other comparisons because it is more sensitive to small parameter changes than other calculations, such as radiative transfer or total emissivity. The calculation method of the ALBDF will be described in detail in Section 4.1. It was found through this study that the ALBDF calculated using the Voigt profile generally lies below the ALBDF calculated using the Lorentz profile for the conditions where Doppler broadening is significant, as mentioned above. Where Doppler broadening is not significant the Voigt profile yields identical results to the Lorentz profile. For example, at a gas temperature of 3000 K the ALBDF calculated using the Voigt profile was less than that calculated using the Lorentz profile by up to about 0.02 for both H$_2$O and CO$_2$. Since the full range of the ALBDF is 1, this can be considered a 2% change.

Rigorously, to obtain the spectral absorption cross-section, $C_\eta(p,T,Y_i)$, the contributions from all lines in the spectrum, $C_j(p,T,Y_i)$, are summed at each wavenumber:

$$C_\eta(p,T,Y_i) = \sum_{j=1}^{m} C_{\eta,j}(p,T,Y_i) \quad (3-2)$$

where $m$ is the total number of spectral lines in the database. As will be discussed in greater detail in a section to follow, in practice only the lines which contribute significantly to the spectral absorption cross section $C_\eta(p,T,Y_i)$ are included in the summation of Eq. (3-2). The spectral absorption coefficient, $\kappa_\eta(p,T,Y_i)$, is then calculated as
\[ \kappa_{\eta}(p, T, Y_i) = N(p, T) Y_i C_{\eta}(p, T, Y_i), \]  

where the mole fraction \( Y_i = p_i/p \) and the gas molar density \( N(p, T) = p N_A / R_u T \). In the latter relation, \( N_A \) is Avogadro’s number and \( R_u \) is the universal gas constant.

Each of the three terms on the right-hand-side of Eq. (3-3) has a dependence on total pressure. However, it may be seen that the product of the molar density, \( N(p, T) \), and the mole fraction, \( Y_i = p_i/p \), is dependent only on the partial pressure. Thus, the dependence of the spectral absorption coefficient, \( \kappa_{\eta}(p, T, Y_i) \), on total pressure is felt exclusively through the influence of total pressure on the absorption cross-section \( C_{\eta}(p, T, Y_i) \). The molar density is calculated using the ideal gas law, as shown above. There is some slight error introduced for water vapor at a combination of low temperature and high pressure when using the ideal gas law (Çengel and Boles, 2006), but it is overall a good approximation for the temperatures and pressures explored in this study. The total pressure dependence of the absorption cross-section is felt through the Lorentz half-width, \( \gamma_L(p, T) \), and to a lesser extent, through the line location, \( \eta_0(p) \), which are calculated as shown below.

The data in HITEMP 2010 are tabulated at the reference temperature of \( T_0 = 296 \) K, and therefore must be scaled to the temperature of interest. Line intensity, \( S(p, T) \), was calculated as follows (Rothman et al., 1998):

\[
S(p, T) = S(T_0) \frac{Q(T_0)}{Q(T)} \exp \left[ \frac{hcE^*}{k} \left( \frac{1}{T_0} - \frac{1}{T} \right) \right] \frac{1 - \exp\left[ -hc\eta_0(p)/kT \right]}{1 - \exp\left[ -hc\eta_0(p)/kT_0 \right]}.
\]  

\[ (3-4) \]

The internal partition function, \( Q(T) \), is taken from information accompanying the 2008 HITRAN database (Rothman et al., 2009). More accurate partition functions for H\(_2\)O may be found in Vidler and Tennyson (2000), but it has been confirmed here that the results of the Vidler and Tennyson study yield partition function ratios, \( Q(T_0)/Q(T) \), that are at most 1.1%
different from those calculated using HITRAN over the full range of temperature investigated in this study. Therefore, the HITRAN partition functions were used in this work for all three species. The partition functions of the primary isotopologue will be used for all isotopologues. This can be justified because the primary isotopologue has an abundance near 99% and because the ratio $Q(T_0)/Q(T)$ varies only slightly from one isotopologue to the next even if the value of $Q(T)$ changes significantly (Rivière and Soufiani, 2012). The values for line intensity at the reference temperature, $S(T_0)$, and lower-state energy, $E''$, are obtained from the HITEMP 2010 database for each spectral line. Line location may experience a shift due to changes in total pressure (Rothman et al., 1998), and is calculated as
\[
\eta_0(p) = \eta_{\text{vac}} + p\delta.
\] (3-5)
Here, the pressure-induced shift in line location, $\delta$, and the line location at vacuum, $\eta_{\text{vac}}$, are found in the HITEMP 2010 database. As can be seen in Eq. (3-4), the line intensity has only a weak dependence upon total pressure through the line location $\eta_0(p)$.

The line half-width at half-maximum was also shifted to the temperature and pressure of interest from the reference temperature (296 K) and pressure (1 atm). For collision broadening this was calculated as (Ludwig et al., 1973; Rothman et al., 1998)
\[
\gamma_L(p, T) = p \left( \frac{T_0}{T} \right)^{n_{\text{air}}} \left[ \gamma_{\text{air}}(1 - Y_i) + \gamma_{\text{self}} Y_i \right]
\] (3-6)
where the coefficient of temperature dependence for air-broadening, $n_{\text{air}}$, and the line half-widths at half-maximum for air- and self-broadening, $\gamma_{\text{air}}$ and $\gamma_{\text{self}}$, were taken from the HITEMP 2010 database. The commonly used approximation that $n_{\text{air}} = n_{\text{self}}$ (Rothman et al., 1998; Zhang, 2002; Chu et al., 2011) was employed in this study, as seen in Eq. (3-6). This approach was adopted because the parameter $n_{\text{self}}$ is not found in the HITEMP 2010 database, and only scant data for $n_{\text{self}}$ exist in the literature, applicable to only a small number of the spectral lines considered in
these calculations. An alternate approach is to apply the classical value of \( n_{\text{self}} = 0.5 \) (Ludwig et al., 1973). \( p \) is the total pressure, and the reference pressure, \( p_0 \), is atmospheric pressure. Doppler broadening depends principally on temperature (with the pressure effect manifested only through a shift in line location given by Eq. (3-5)), and is calculated as (Modest, 2003)

\[
\gamma_D(p, T) = \frac{n_0(p)}{c} \sqrt{\frac{2kT}{M_i}} \ln 2. \tag{3-7}
\]

Only lines with a significant impact on ALBDF results were included in the line-by-line calculations. Weaker lines were not included in the generation of the absorption spectrum, \( C_p(p, T, Y_i) \). It was determined that a line intensity cutoff value of \( 10^{-26} \text{ cm}^{-1}/(\text{molecule } \times \text{ cm}^2) \) was sufficient for CO at all temperatures, and for H\(_2\)O at temperatures below 2500 K. A cutoff value of \( 10^{-27} \text{ cm}^{-1}/(\text{molecule } \times \text{ cm}^2) \) was required for CO\(_2\) at all temperatures, and for H\(_2\)O at temperatures of 2500 K and above. Decreasing these cutoff values by a factor of 10 resulted in a maximum change in the ALBDF of less than 0.01 (\( \text{i.e.} \), less than 1\%). It was found that the ALBDF at high temperatures was the most sensitive to this change. Figure 3.1 shows the ALBDF for CO\(_2\) at \( T_g = T_b = 3000 \text{ K} \) calculated using line intensity cutoff values ranging from \( 10^{-24} \) to \( 10^{-28} \text{ cm}^{-1}/(\text{molecule } \times \text{ cm}^2) \). As can be seen, the ALBDF converges to an unchanging value for all absorption cross-section with a cutoff value of \( 10^{-27} \text{ cm}^{-1}/(\text{molecule } \times \text{ cm}^2) \).

The number of lines included in calculations based on the cutoff criteria specified for the three species for various temperatures between 400 and 3000 K is shown in Fig. 3.2 for a) H\(_2\)O and CO\(_2\), and b) CO. As can be seen, the number of contributing CO\(_2\) lines does not always increase with temperature, and in fact reaches a maximum value near 8.6 million at 2200 K. Some spectral lines have a very low value of lower-state energy, \( E'' \). When this value is low
Figure 3.1: The ALBDF of CO$_2$ at $T_g = T_b = 3000$ K and $p = 1$ atm. Intensity cutoff values ranging from $10^{-24}$ to $10^{-28}$ cm$^4/(molecule \times cm^2)$ are shown for comparison.

Figure 3.2: The number of spectral lines included in calculations for a) H$_2$O, CO$_2$, and b) CO as a function of temperature.
enough the intensity of a line can decrease as temperature increases. By contrast, the numbers of contributing lines for both H₂O and CO increase monotonically with temperature. Because the cutoff value for H₂O is reduced at 2500 K, a large jump is observed at this temperature. The number of significant lines reaches 60 million for H₂O and almost 25 thousand for CO at the maximum temperature considered here, 3000 K.

The absorption cross-section, \( C_\eta(p,T,Y_i) \), as calculated using Eq. (3-2) requires that the contribution from each line, \( C_\eta(p,T,Y_i) \), be included at every spectral location. However, including all lines in the generation of the absorption spectrum is both unnecessary and computationally expensive. Further, it has been well established that the Lorentz line profile, which is the dominant element of the Voigt line profile for the conditions explored in this study, over-predicts the absorption cross-section in the far-wing regions of the line (Mlawer et al., 2012; Perrin and Hartmann, 1989). As mentioned in Chapter 2, these studies propose a factor, \( \chi \), to correct the line shape to match experimental data more closely. However, the MT-CKD model of Mlawer et al. (2012), which corrects the line shape of H₂O, has only been developed for applications near room temperature and atmospheric pressure (Mlawer et al., 2012), and a recent paper suggests that the MT-CKD model under-predicts \( C_\eta(p,T,Y_i) \) in the spectral window regions (Ptashnik et al., 2013). Nevertheless, the MT-CKD model gives the best available correction to the Lorentz profile for H₂O. The \( \chi \) factor for CO₂ is applicable to temperatures as high as 800 K and for pressures ranging from 0 to 60 bars (Perrin and Hartmann, 1989).

Until more data become available at the elevated temperatures and pressures investigated in this study, the following procedure was used: the average number of line half-widths was calculated for which the Lorentz profile yields data that is within an order of magnitude of the corrected line shape (using either the MT-CKD model for H₂O or the model developed by Perrin
and Hartmann for CO₂) at the highest temperature and pressure for which the corrected profile is valid, and this number of half-widths was used as the line wing cutoff for all temperatures and pressures. For H₂O this calculation was performed at $T = 300$ K and $p = 1$ atm while for CO₂ it was carried out at $T = 800$ K applicable to all total pressures considered in this work since the $\chi$ factor for CO₂ does not depend on pressure but was found to apply to the total pressure range $0 < p < 60$ atm (Perrin and Hartmann, 1989). The line half-widths from Rivière and Soufiani (2012) were used in this calculation, and a single line wing cutoff was chosen for all mole fractions of the species of interest. Based on this calculation, the line wing cutoff used was 2750 half-widths for H₂O, and 600 half-widths for CO₂. Because no correction factor data are available for CO, the same cutoff criterion used for CO₂ was also applied to CO since the two species generally demonstrate similar behavior.

Figure 3.3 demonstrates the application of the above process to H₂O at 300 K in the limit of air-broadening only ($Y_{H₂O} \to 0$). The generic absorption cross-section calculated using the Lorentz profile and using the MT-CKD model are plotted as a function of distance from the line center in cm⁻¹. As can be seen, the Lorentz profile has a smaller magnitude near the line center but a much higher magnitude in the far-wing region – approximately four orders of magnitude higher a distance of 250 cm⁻¹ from the line center. The difference at the line center has a negligible impact on calculations because the peak is very narrow. The line wings, although reaching a smaller magnitude than the peak, have a much stronger impact on calculations because they cover a large spectral distance. At a spectral spacing 153 cm⁻¹ from the line center, the Lorentz profile gives an absorption cross-section that is a factor of 10 higher than that predicted using the MT-CKD model. This corresponds to about 2190 half-widths according to the average half-width reported by Rivière and Soufiani (2012) for pure air-broadening of H₂O.
lines at 300 K and 1 atm. This value was averaged with 3310, the value obtained when a medium of pure H$_2$O ($Y_{H_2O} = 1$) is considered, resulting in 2750 half-widths to be used as a cutoff for the line wings of H$_2$O. For the data given in Fig. 3.3, this corresponds to a distance of 192 cm$^{-1}$ from the line center, although the actual cutoff distance in cm$^{-1}$ depends on temperature and pressure.

![Figure 3.3: The absorption cross-section, $C$, as a function of distance from line center in cm$^{-1}$ calculated using the Lorentz profile and the MT-CKD model.](image)

To further minimize computational effort, line wings should be included in the summation of Eq. (3-2) at all spectral locations where they maintain a non-negligible contribution to $C_i(p,T,Y)$, similar to a process mentioned by Modest and Singh (2005). The investigation to determine an appropriate cutoff value began with a value of $10^{-34}$ cm$^2$/molecule, and the cutoff value was systematically increased until the resulting change to the ALBDF was significant over the range of $C$ explored in this study ($C_{\text{min}} = 5 \times 10^{-25}$ cm$^2$/molecule for all species; $C_{\text{max}} = 10^{-18}$ cm$^2$/molecule for H$_2$O and CO, $C_{\text{max}} = 10^{-17}$ cm$^2$/molecule for CO$_2$). As the
cutoff value was increased from a value of \(10^{-34}\) cm\(^2\)/molecule the change in ALBDF was first manifested at the lowest value of \(C\), where the impact on radiative transfer is weakest. A cutoff value of \(10^{-29}\) cm\(^2\)/molecule was thus chosen, at which point the maximum change in ALBDF compared to using a cutoff of \(10^{-34}\) cm\(^2\)/molecule was found to be less than 0.2%.

The method of applying the cutoff value to the line wings will now be described. The entire gas absorption spectrum (0 to 25,000 cm\(^{-1}\)) was divided into discrete wavenumbers, with the wavenumber interval defined here by \(\Delta \eta = 0.005\) cm\(^{-1}\) (yielding 5 million discrete wavenumbers for the spectral range 0 to 25,000 cm\(^{-1}\)). The value of \(C_\eta\) was initialized to 0 at all discrete wavenumbers. The set of applicable lines was then considered individually at each wavenumber. The contribution of each spectral line was included first at the line center, and then its contribution to wavenumbers moving in the positive and negative wavenumber directions were added until they fell below the cutoff value of \(10^{-29}\) cm\(^2\)/molecule or until the number of half-widths from the line center exceeded the cutoff value associated with Lorentz line applicability for the species of interest (2750 half-widths for H\(_2\)O and 600 half-widths for CO\(_2\) and CO).

An alternate method for discretizing with respect to wavenumber is to first choose the location of every spectral line at the temperature of interest. Next, the space between lines is divided into a systematically increasing number of intervals (i.e., successively finer resolution) until any subsequent calculations (such as those described in Chapter 4) become independent of the number of spectral intervals. This method is, most strictly speaking, the true line-by-line approach. However, it is significantly more computationally expensive and, as confirmed in this study, yields identical results to the method of using evenly spaced wavenumbers. As an illustration, the true line-by-line approach requires approximately 20 spectral intervals between
line locations before ALBDF calculations cease to change with further decreases in the number of spectral intervals. Discretizing the spectrum with 20 intervals between lines results in 9,845,400 discrete wavenumbers for the case of H$_2$O at the relatively low temperature of 1000 K. By contrast, the evenly spaced discretization method described previously requires only 5 million discrete wavenumbers for any temperature. Therefore, the evenly spaced discretization approach was applied for all calculations of the absorption cross-section.

The absorption cross-section was calculated from the line-by-line spectral database for wavenumbers between 0 and 25,000 cm$^{-1}$, or up to the point where no lines give a significant contribution according to the criteria described above. The HITEMP 2010 database does not include lines for CO$_2$ above $\eta = 12785$ cm$^{-1}$ or for CO above $\eta = 8465$ cm$^{-1}$. At 3000 K, 99.8% of the total blackbody emissive power is accounted below this wavenumber maximum. For lower temperatures, the wavenumber maximum 25,000 cm$^{-1}$ is much higher than is needed to capture all of the emissive power. Figure 3.4 shows the effect of temperature on the distribution of the Planck blackbody emissive power, and is a plot of the spectral Planck blackbody emissive power, $E_{\eta}$, normalized by the maximum emissive power, $E_{\text{max}}$, as a function of wavenumber at temperatures ranging from 500 K to 3000 K. As can be seen, the range of wavenumbers needed to capture the full emissive power increases significantly with temperature, and at 3000 K, a wavenumber range up to 25,000 cm$^{-1}$ is required.

It might be noted that the method of generating the absorption cross-section described above and adopted here differs from that used by Denison and Webb (1993b, 1996a) in that here, the updated HITEMP 2010 database is used, the more general Voigt line profile is employed, a broader wavenumber range is included in the calculations, and a more rigorous method for accounting for line contributions to $C_{\eta}(p,T,Y_i)$ is formulated. Further, the absorption spectrum for
CO has been generated, the total pressure dependence is characterized for all three gas species here, and all three species are studied over a wider temperature range.

Figure 3.4: The spectral emissive power normalized by the maximum emissive power, $E_\eta/E_{\text{max}}$, as a function of wavenumber for temperatures ranging from 500 K to 3000 K.

The absorption cross-section as a function of wavenumber is shown in Fig. 3.5 for total pressures of 0.1, 1, 8, and 50 atm for a) H$_2$O, b) CO$_2$, and c) CO at 1500 K. The panels on the left show the full spectrum from 0 cm$^{-1}$ up to a wavenumber of nominally 9000 cm$^{-1}$, while the graphs on the right illustrate a small portion of the spectrum at high resolution near 2000 cm$^{-1}$. It can be seen that the effect of increasing total pressure is to smooth the absorption cross-section behavior, rendering the radiation characteristics more continuous in the spectrum. The line peaks are lowered while the line wings increase in strength as total pressure is increased. This is particularly apparent in the full spectrum graphs (left panels) for each species, where it can be seen that for CO$_2$ and CO there are large windows between the primary vibration-rotation bands.
Figure 3.5: Absorption cross-section as a function of wavenumber for a) H$_2$O, b) CO$_2$, and c) CO at 1500 K. The panel on the left shows the data for the full spectrum, while the panel on the right shows a small portion (3 cm$^{-1}$ wide) near 2000 cm$^{-1}$. Total pressures of 0.1, 1, 8, and 50 atm are represented.
that are strongly affected by pressure changes at high total pressure. The absorption cross-section increases significantly in these regions as pressure increases. The lines broaden because the Lorentz line half-width is proportional to pressure. The shift in line location due to pressure given by Eq. (3-5) has an imperceptible effect on the absorption cross-section data for H₂O and CO₂. No shift in line location is included for CO since the tabulated value of δ in the HITEMP 2010 database for this species is zero for all lines.

The spectral absorption data generated using the method described in the foregoing sections were also compared to low-temperature experimental data obtained from Ptashnik et al. (2013) for pure water vapor. Figure 3.6 shows this comparison for a) 289 K, and b) 318 K. The experimental data were accompanied by a margin of error in the publication, and Fig. 3.6 shows the minimum and maximum values based on this margin. It appears that the experimental data at the top of the bands are below the calculated values, but this can be attributed to the fact that the limited resolution of the experimental data does not allow it to capture the very narrow peaks. The experimental data in the valleys show some disagreement with the calculated values for the 289 K case, but the agreement is excellent for the slightly higher temperature case. Further, the valleys behave effectively as spectral windows in radiative transfer calculations, and the contribution of absorption cross-section below a threshold is minimal. Overall, the line-by-line solution obtained from HITEMP 2010 has good agreement with the experimental data.

3.3 Mixtures of Gases

For many practical applications, the absorption cross-section spectrum for a mixture of gases is required. This is obtained by a mole fraction-weighted sum of the cross-sections from all individual species, as given by the following equation (Solovjov and Webb, 2000):
Figure 3.6: The absorption cross-section, $C_{\eta}$, as a function of wavenumber, $\eta$, at a) 289 K and b) 318 K. Shown are the LBL solution generated using the present method and the experimental data from Ptashnik et al. (2013). The minimum and maximum values of the experimental data are shown, based on the margin of error for the data.
\[ C_{\text{mix}, \eta} = Y_1 C_1 \eta + Y_2 C_2 \eta + \cdots + Y_m C_m \eta, \]  

(3-8)

The mixture of gases may then be treated as a single gas with absorption spectrum \( C_{\text{mix}, \eta} \). A requirement of this equation is that the spectral discretization must be the same for each of the species considered in all spectral calculations (e.g., generation of the ALBDF). It should be further noted that rigorously, the absorption cross-section depends on pressure, temperature, and mole fraction differently for each species in the mixture. The mixture spectral absorption cross-section given by Eq. (3-8) must therefore be generated at each thermodynamic state of interest.

When dealing with mixtures of gases, the line broadening caused by collisions with other species present should be considered. The HITEMP 2010 database only contains data for line broadening due to self- and air-broadening. The data for broadening caused by the presence of species other than air and the species of interest are not included in the HITEMP 2010 database, and there is only scant data in the literature characterizing this behavior. However, the average number of half-widths reported by Rivière and Soufiani (2012) account for the presence of other species and can be employed to determine the overall importance of broadening by other species.

The effect of broadening by H\(_2\)O and CO\(_2\) on the ALBDF of CO will demonstrate the importance of accounting for the presence of other species. Carbon monoxide is of particular interest because it is typically only present when H\(_2\)O or CO\(_2\) are present. Because of this, it will be used to examine the effect of broadening by other species. For CO, the effects of self- and air-broadening are nearly identical, so the influence of broadening by other species is readily apparent. The average CO line half-width is given by the following equation (Rivière and Soufiani, 2012):

\[
\tilde{\gamma}_{\text{CO}} = \frac{p}{p_0} \left\{ 0.075 Y_{\text{CO}_2} \left( \frac{T_0}{T} \right)^{0.6} + 0.06 (1 - Y_{\text{CO}_2} - Y_{\text{H}_2\text{O}}) \left( \frac{T_0}{T} \right)^{0.7} + 0.12 Y_{\text{H}_2\text{O}} \left( \frac{T_0}{T} \right)^{0.82} \right\}. 
\]  

(3-9)
As can be seen, this parameter depends on the mole fractions of CO\textsubscript{2} and H\textsubscript{2}O, but not CO. This is because the line half-widths for self-broadening are nearly identical to the half-widths due to air-broadening.

Although the formal definition of the ALBDF and the method of its calculation will be presented in the following chapter, some ALBDF data are given here to more clearly illustrate the effect of broadening on the ALBDF by other species. Figure 3.7 shows the ALBDF for CO in the presence of different concentrations of a) H\textsubscript{2}O, and b) CO\textsubscript{2}, incorporating Eq. (3-9). The remaining gas present in the mixture is air. Shown are data for $T_{g} = T_{b} = 400$ K, 1700 K, and 3000 K at a total pressure of 1 atm. As can be seen, as the mole fraction of H\textsubscript{2}O or CO\textsubscript{2} increases, there is a small change in the ALBDF of CO that is slightly more pronounced for the case of H\textsubscript{2}O. However, this change is small enough in all cases that it can be neglected without a significant loss of accuracy. It is interesting to note that the ALBDF for CO for the case of air-broadening only calculated using Eq. (3-9) is at most 0.5% different from the ALBDF calculated using the half-widths in the HITEMP 2010 database (not shown on Fig. 3.7).

Self-broadening has been shown to exert a significant influence on the ALBDF of H\textsubscript{2}O (Denison and Webb, 1993b; Pearson et al., 2013a). It was found that self-broadening was the most significant source of collision broadening for H\textsubscript{2}O even with the inclusion of other species. Therefore, all other species present can be treated as air. For CO\textsubscript{2}, the contribution to line broadening by other species is similar to the case of CO.

Based on this investigation, it has been determined that the line broadening due to collisions with other species can be neglected. Although the ALBDF experiences a change when other species are included in line broadening calculations, the change is relatively small. Further, the complication of adding more variables to the correlation of the ALBDF is not justified by so
small a change. Therefore, all calculations of the absorption cross-section will assume only air- and self-broadening, with other species present being treated as air for the calculation of line broadening.

![Figure 3.7: The ALBDF, $F$, of CO as a function of absorption cross-section, $C$, for three temperatures and three values of mole fraction of a) CO$_2$ and b) H$_2$O, as shown. For all cases, $T_g = T_b, p = 1$ atm, $Y_{CO} \to 0$.](image-url)
3.4 Summary

The method of generating the line-by-line spectral absorption cross-section has been described in detail in this chapter. The HITEMP 2010 database is used to generate the absorption spectrum. Because of its better accuracy at the range of conditions investigated here, the Voigt line profile has been employed. The contribution of a given spectral line is added to all spectral locations where it has a significant contribution, based on its half-width at half-maximum. A cutoff value that determines when a line is no longer significant has been applied. Further, a cutoff value determining which lines are not sufficiently strong to contribute to the resulting data has been applied. Because the Lorentz line profile, the dominant element of the Voigt profile for the conditions in this study, is known to lose accuracy in the far-wing region, line wings are restricted to a certain distance from the line center. This distance was determined using models that are based on empirical data for limited thermodynamic conditions. The method of extending the development to mixtures of participating gases has also been described. This method includes a summation of the contributions to the absorption cross-section of each gas in the mixture weighted by its mole fraction such that the mixture can be treated as a single gas. The effect of line broadening due to other species has been examined. Based on this study, it has been concluded that the line broadening by other gases present can be treated as air-broadening with little loss of accuracy.
4 TOTAL PRESSURE EFFECTS ON RADIATIVE TRANSFER

After generating the line-by-line (LBL) absorption cross-section data as described in Chapter 3, calculations for other parameters based on the detailed absorption spectrum can be obtained. This chapter will describe the generation of LBL representations of the absorption line blackbody distribution function, total emissivity, the Planck mean absorption coefficient, and predictions for radiative transfer in a one-dimensional layer of gas. These LBL solutions will be used for three purposes. First, they will be used in the present chapter to explore the effects of variable total pressure on radiative transfer. Second, the ALBDF generated from line-by-line data will be used to produce efficient ALBDF representations in Chapter 5. Finally, the LBL solutions will be used in Chapter 6 as benchmark data to determine the accuracy of the newly proposed representations of the ALBDF.

4.1 The Absorption Line Blackbody Distribution Function (ALBDF)

The absorption line blackbody distribution function (ALBDF) is used in the SLW solution method for radiative transfer to enable integration over absorption coefficient instead of the computationally intensive process of integrating over wavenumber. The number of integrations is thus reduced from millions to typically fewer than 20. The ALBDF is defined as the fraction of blackbody radiative power that is emitted in wavenumber regions where the
spectral absorption cross-section, $C_\eta$, is below a prescribed value $C$, and is represented mathematically as (Denison and Webb, 1993b)

$$F(C, p, T_g, T_b, Y) = \frac{1}{\sigma T_b^4} \int_{\{\eta: c_\eta(p, T_g, Y) \leq C\}} E_{b\eta}(T_b, \eta) d\eta. \tag{4-1}$$

where $T_g$ is the gas temperature, $T_b$ is the blackbody source temperature, $p$ is the total pressure, $Y$ is the mole fraction of the species of interest, and $E_{b\eta}$ is emissive power.

Figure 4.1 depicts graphically how the ALBDF is derived from spectral data and how it changes the integration process. The left side of the figure shows the ALBDF for an arbitrary temperature and concentration with the ALBDF (varying from 1 to 0) on the horizontal axis. The absorption cross-section is on the vertical axis in order to match the right side of the figure, which shows the corresponding spectral absorption cross-section data as a function of wavenumber. An arbitrary portion of the spectrum is shown. Two values of absorption cross-section are shown, $C_i$ and $C_{i-1}$. It can be seen that as $C$ increases, a greater portion of the spectral absorption cross-section falls below the specified value. This corresponds to an increase in the fraction of blackbody power in spectral regions below the prescribed value $C$, or in other words, an increase in the ALBDF, $F$. When all the absorption cross-section data at all wavenumbers are below the prescribed value of $C$, the ALBDF reaches a value of unity. When making calculations of radiative transfer, the spectrum is divided into a prescribed number of “gray gases” between a predetermined minimum and maximum value of $C$. Practically, the minimum and maximum value of $C$ are chosen to effectively capture all radiant energy in a particular application. An arbitrarily chosen gray gas $i$ is shown in Fig. 4.1, corresponding to the lighter shaded region between $C_i$ and $C_{i-1}$. The idea behind global models, such as the SLW model, is to integrate the radiative transfer equation (RTE) once per gray gas, accounting for all regions of the spectrum
where the gas absorbs and emits between $C_i$ and $C_{i-1}$. The spectral regions accounted for by gray gas $i$ are shown by the darker shading on the right side of the figure.

![Figure 4.1](image)

Figure 4.1: The absorption cross-section, $C$, as a function of ALBDF, $F$, is shown on the left graph. The right graph shows the corresponding spectral absorption cross-section data as a function of wavenumber, $\eta$. Gray gas $i$ is the lighter shaded region, corresponding to portions of the spectrum shown by the darker shading.

To compute the ALBDF from line-by-line data, the value of $C_\eta$ for the spectrum generated at a given $T_g$ and $p$ within a small segment of wavenumber $\Delta \eta$ was compared to a specified value, $C$. The value of $C_\eta$ within a given segment was found by averaging the values of $C_\eta$ at the endpoints of the spectral segment. The Planck blackbody energies within the segments where $C_\eta \leq C$ were summed, and the result was divided by the total emissive power at the specified temperature $T_b$. It was found that $\Delta \eta = 0.005 \text{ cm}^{-1}$ was suitable for these calculations, and that further refinement beyond this value did not result in a significant change in the ALBDF over the range of temperature and pressure investigated in this study. For example, using a spectral step of $\Delta \eta = 0.001 \text{ cm}^{-1}$ for CO at $T_g = T_b = 3000 \text{ K}$ and $p = 1 \text{ atm}$, a factor of five
smaller, showed a maximum difference of 0.026% compared to $\Delta \eta = 0.005$ cm$^{-1}$. A similar difference is expected for the conditions in this work. This was the reason for the choice of spectral resolution when generating the spectral absorption cross-section as described in Chapter 3. The code used to calculate the line-by-line ALBDF, as described here, can be found in Appendix B.

Arguably, a more rigorous method of calculating the ALBDF from line-by-line data is to find the actual wavenumber locations where the prescribed value $C$ intersects with the detailed spectral absorption cross-section, $\eta$. In this method, the portions of the spectrum where $\eta < C$ are determined exactly. A computer code was written to apply this method, and it was found that the results were identical to the method employing evenly-spaced spectral intervals described in the previous paragraph, when a fine enough resolution is chosen. This is further justification for the $\Delta \eta = 0.005$ cm$^{-1}$ discretization used. Because of this, and because applying the evenly-spaced approach is simpler and less computationally demanding than this more rigorous approach, the evenly-spaced approach was used for all ALBDF calculations associated with this study.

### 4.1.1 ALBDF of Water Vapor

The absorption cross-section data were used to calculate the ALBDF for each of the three species of interest to this study, H$_2$O, CO$_2$, and CO. Shown in Fig. 4.2 is the ALBDF for H$_2$O at a) $T_g = T_b = 1000$ K, and b) $T_g = T_b = 2500$ K. For Fig. 4.2a, total pressures of 0.1, 0.25, 0.5, 1, 2, 4, 8, 15, 30, and 50 atm are shown. For both temperatures, it can be seen that as total pressure increases, the ALBDF shifts downward. This corresponds to an increase in the absorption of the gas caused by the stronger line broadening at higher total pressure. When the spectral lines are wider, the regions between line peaks are raised, resulting in more absorption. It can be seen that
at 1000 K the ALBDF is more sensitive to changes in total pressure at low pressure; the total pressure change from 0.1 atm to 0.25 atm has a similar quantitative effect on the ALBDF as the much more significant change from 8 atm to 50 atm.

![Graph showing ALBDF, F, as a function of absorption cross-section, C, for H2O at a) Tg = Tb = 1000 K, and b) Tg = Tb = 2500 K for total pressures varying from 0.1 atm to 50 atm as shown. Data are shown for the limit of approaching zero mole fraction of H2O.]

It is also surprising to note that the ALBDF becomes less smooth as total pressure increases, even though the spectral absorption cross-section becomes smoother. An explanation for this behavior is found when the definition of the ALBDF is considered. The ALBDF is the fraction of emissive power in spectral regions where the spectral absorption cross-section, \( C_\eta(p,T,Y_i) \), is less than the arbitrary value of \( C \). When the spectral lines are narrower and taller (as is the case at lower total pressure), the change in the ALBDF as \( C \) increases is gradual. When the lines are wider with lower peaks, an increase in \( C \) leads to more abrupt changes in the ALBDF. This can be observed in the left panels of Fig. 3.3 where a change in \( C \) results in a more abrupt change in the portion of the absorption cross-section data that lie below \( C \).
As can be seen in Fig. 4.2b, changes in total pressure have a smaller impact on the ALBDF at elevated gas temperatures. As gas temperature increases the density of spectral absorption lines is higher, so the effect of increasing pressure is diminished. Again it is seen that the ALBDF is smoother for lower pressures.

As mentioned in Section 3.3, all other parameters remaining the same, the mole fraction of H$_2$O has a significant impact on the ALBDF. Figure 4.3 illustrates the ALBDF as a function of absorption cross-section at $T_g = 1000$ K, and $T_b = 1000$ K or 2500 K for H$_2$O mole fraction extremes of approaching 0 and equal to 1. For both values of $T_b$, it can be seen that a change of mole fraction at 1 atm total pressure results in a shift in the ALBDF to lower $F$ that is similar for all values of absorption cross-section. However, at 50 atm, the shift is stronger for lower values in absorption cross-section than at higher values, although the overall effect is similar to the atmospheric pressure case.

Figure 4.3: The ALBDF, $F$, as a function of absorption cross-section, $C$, for H$_2$O mole fractions of approaching 0 and equal to 1. The data is given at total pressures of 1 atm and 50 atm as shown. $T_g = 1000$ K, and $T_b = 1000$ K or 2500 K as shown.
4.1.2 ALBDF of Carbon Dioxide

Figure 4.4 illustrates the line-by-line-generated ALBDF as a function of absorption cross-section for CO$_2$ at a) $T_g = T_b = 1000$ K, and b) $T_g = T_b = 2500$ K. For the lower temperature case (Fig. 4.4a) eight total pressures varying between 0.1 and 50 atm are shown. It can be seen that the ALBDF shifts to lower values as total pressure increases, similar to what was seen with the ALBDF for H$_2$O. However, for CO$_2$, the shift is quite weak at values of absorption cross-section above approximately $10^{-21}$ cm$^2$/molecule. The shift at lower values of absorption cross-section is much stronger. This uneven shift with absorption cross-section is likely caused by the wider windows between vibration-rotation bands in the CO$_2$ spectrum evident in the left panel of Fig. 3.3b. Unlike H$_2$O, the ALBDF for CO$_2$ exhibits more sensitivity to pressure changes at high total pressure than at low pressure, although this increased sensitivity is seen primarily at low absorption cross-section and low temperature.

The ALBDF of CO$_2$ shows that, in general, CO$_2$ is less absorbing than H$_2$O. This can be seen in the lower slope of the ALBDF and because the value of $F$ at the minimum value of $C$ is often near 0.4 instead of near zero as is the case for the ALBDF of H$_2$O. The reason for the higher value of $F$ at the minimum value of $C$ is that CO$_2$ has much stronger spectral windows than H$_2$O, and the ALBDF of CO$_2$ is affected by these non-absorbing regions in this manner.

For the ALBDF of CO$_2$ at high temperature (Fig. 4.4b) the effect of total pressure is similar to the case of water vapor in that the ALBDF doesn’t change as significantly as total pressure increases as it does in the low temperature case. Also, it is interesting to note that the ALBDF of CO$_2$ is much less smooth than it is for H$_2$O, the result of narrower absorption bands.
Figure 4.4: The ALBDF, $F$, as a function of absorption cross-section, $C$, for CO$_2$ at a) $T_g = T_b = 1000$ K, and b) $T_g = T_b = 2500$ K for total pressures varying from 0.1 atm to 50 atm as shown. Data are shown for the limit of approaching zero mole fraction of CO$_2$.

It has previously been noted that a change in mole fraction of CO$_2$ results in a negligible change in the ALBDF (Denison and Webb, 1995a; Modest and Mehta, 2004). This has been confirmed using the HITEMP 2010 spectral database over the range of total pressure investigated in this study. Figure 4.5 shows the ALBDF of CO$_2$ as a function of absorption cross-section for mole fractions of CO$_2$ of approaching 0 and equal to 1 at pressures of 1 and 50 atm, and $T_g = 1000$ K and $T_b = 1000$ K or 2500 K, as shown. As can be seen, the slight shift to lower ALBDF for pure CO$_2$ compared to the limit of air broadening only evident at 50 atm, though larger than the shift at atmospheric pressure, is still very weak. The dependence of ALBDF on mole fraction for CO$_2$ can thus be safely neglected, since the largest possible effect of increasing mole fraction from approaching zero up to one (for the range of parameters considered in this study) only causes a shift in the ALBDF of 0.4% on average.
4.1.3 ALBDF of Carbon Monoxide

The ALBDF of CO has also been calculated from line-by-line data. Figure 4.6 shows the ALBDF of CO as a function of absorption cross-section for a) $T_g = T_b = 1000$ K, and b) $T_g = T_b = 2500$ K. The ALBDF for CO is similar to that of CO$_2$ for the lower temperature case (Fig. 4.6a), with a much stronger pressure-induced shift at lower values of absorption cross-section. The same weaker shift due to total pressure at high temperature that was apparent for H$_2$O and CO$_2$ is also evident for CO, as can be seen in Fig. 4.6b. The ALBDF data for CO begin at an even higher value at the minimum value of $C$ than CO$_2$ with an even lower slope, which suggests that CO has weaker absorption of energy than either CO$_2$ or H$_2$O.

The impact of self-broadening on the ALBDF for CO is less significant even than it is for CO$_2$, so graphs illustrating this are not shown. This was found to be the case for all total pressures.
Figure 4.6: The ALBDF, $F$, as a function of absorption cross-section, $C$, for CO at a) $T_g = T_b = 1000$ K, and b) $T_g = T_b = 2500$ K for total pressures varying from 0.1 atm to 50 atm as shown. Data are shown for the limit of approaching zero mole fraction of CO.

4.1.4 Comparisons with Previous Work

The line-by-line ALBDF generated using the HITEMP 2010 data will now be compared to benchmark line-by-line ALBDF calculations from Denison (1994). This comparison will illustrate the importance of providing improved representations of the ALBDF, one of the objectives of this work. Figure 4.7 shows the ALBDF of $\text{H}_2\text{O}$ at $p = 1$ atm and $Y_{\text{H}_2\text{O}} \to 0$ for a) $T_g = 1000$ K and $T_b = 500$, 1500, and 2500 K, and b) $T_b = 1000$ K and $T_g = 500$, 1500, and 2500 K. Shown are new line-by-line results calculated from HITEMP 2010 and those reported by Denison (1994). As can be seen, the updated spectral data significantly affects the ALBDF of $\text{H}_2\text{O}$. The newer data lie below the data of Denison which can be attributed to the significantly expanded spectral database employed. As more lines are added to the spectrum, the overall spectral absorption cross-section, $C\eta$, increases in strength. As a result, the ALBDF decreases in...
magnitude because a smaller fraction of the absorption spectrum is below the prescribed value, $C$. Because most of the lines added to the spectral database are for elevated temperatures, the effect on low temperature calculations is much smaller, as can be seen at a gas temperature of 500 K (Fig. 4.7b).

Comparisons of ALBDF data generated using the previous and updated spectral database for CO$_2$ were also made. Figure 4.8 shows the ALBDF of CO$_2$ calculated using HITEMP 2010 and that reported by Denison (1994). The data are for $p = 1$ atm and $Y_{CO_2} \rightarrow 0$ for a) $T_g = 1000$ K and $T_b = 500, 1500, \text{ and } 2500$ K, and b) $T_b = 1000$ K and $T_g = 500, 1500, \text{ and } 2500$ K. This comparison reveals that the newer spectral data do not change the ALBDF of CO$_2$ as much as was observed for H$_2$O, especially at high absorption cross-section, where the previous work and the present work appear to coincide.
Figure 4.8: The ALBDF of CO$_2$ at $p = 1$ atm and $Y_{CO_2} \to 0$ for a) $T_g = 1000$ K and $T_b = 500$, 1500, and 2500 K, and b) $T_b = 1000$ K and $T_g = 500$, 1500, and 2500 K. Calculations from Denison (1994) and the ALBDF calculated using HITEMP 2010 are shown.

4.2 The Planck-Mean Absorption Coefficient

The Planck-mean absorption coefficient, $\kappa_p$, can be used in evaluation of total intensity or the divergence of flux and is defined as (Modest, 2003)

$$\kappa_p = \frac{\int_0^\infty I_{bn} \kappa_\eta d\eta}{\int_0^\infty I_{bn} d\eta}$$  \hspace{1cm} (4-2)

This quantity can be calculated directly using the HITEMP 2010 database. This was done according to the expression developed previously (Zhang and Modest, 2002):

$$\kappa_p = \sum_j \left( \frac{\pi I_{bn,j}}{\sigma T^4} \right) S_j.$$  \hspace{1cm} (4-3)

49
In this expression, $I_{b\eta,j}$ is the radiative intensity and $S_j$ is the line intensity of the $j$th spectral line. The summation is carried out over all lines that contribute in a significant way (as defined in Chapter 3) for the temperature of interest. The Planck-mean absorption coefficient is independent of pressure (Modest, 2003), and thus this parameter was calculated using atmospheric data only. Figure 4.9 shows the Planck-mean absorption coefficient as a function of temperature using the line-by-line formulation and a correlation based on the RADCAL software (Grosshandler, 1993; Barlow et al., 2001). The RADCAL formulation is experimentally based, and the excellent agreement between the LBL results and the correlation based on RADCAL, particularly for H$_2$O and CO, suggests that the HITEMP 2010 database gives an accurate description of the spectral properties of these species. Some disagreement is seen for CO$_2$. This is not surprising since the original formulation of RADCAL encountered particular difficulty in predicting CO$_2$ behavior (Grosshandler, 1993).

Figure 4.9: The Planck-mean absorption coefficient, $\kappa_p$, as a function of temperature for H$_2$O, CO$_2$, and CO. Shown are the line-by-line data and the calculation using the correlation based on RADCAL (Grosshandler, 1993; Barlow et al., 2001).
4.3 Total Emissivity at Variable Pressure

The total emissivity, $\varepsilon(p,T,L)$, was calculated as a function of total pressure using the line-by-line data from its definition as

$$\varepsilon(p,T,L) = \sum_{j=1}^{m} f_j (1 - e^{-\kappa_j(p,T)L}),$$

(4-4)

where $L$ is the pathlength and $m$ is the total number of wavenumber intervals in the spectrum to be included in the summation. The absorption coefficient, $\kappa_j(p,T)$, was calculated according to Eq. (3-3) within each wavenumber interval as the average of the values at the endpoints of each interval, and $f_j$ is the fraction of blackbody emissive power contained within that interval. Wavenumber intervals were again set to $\Delta \eta = 0.005 \text{ cm}^{-1}$ and covered the spectral region $0 < \eta < 25,000 \text{ cm}^{-1}$.

Figure 4.10 shows the total emissivity as a function of temperature for a) H$_2$O, b) CO$_2$, and c) CO. For the data shown, the pathlength is $L = 1 \text{ m}$, mole fraction is $Y_i = 0.01$, total pressure was varied from 0.1 atm to 50 atm, and temperature was varied from 400 K to 3000 K. The solid lines represent total emissivity calculated using the detailed spectral data obtained from HITEMP 2010, and the dashed lines were calculated using the Leckner correlation, which is available only for H$_2$O and CO$_2$ (Leckner, 1972, Modest 2003). As can be seen, increasing the total pressure results in a significant change in emissivity for H$_2$O, CO$_2$, and CO. Further, for H$_2$O and CO$_2$, the emissivity calculated using the detailed spectral data compares favorably with the Leckner correlation, which, although dated, is experimentally based (Leckner, 1972). There are some regions where the comparison shows discrepancy, principally at lower temperatures.
Figure 4.10: Total emissivity as a function of temperature for a) H2O, b) CO2, and c) CO for \( Y_i = 0.01 \) (unless otherwise noted), \( L = 1 \) m, and total pressure as shown. Solid lines represent line-by-line predictions and dashed lines represent the Leckner correlation.

An important parameter in the calculation of total emissivity is the product of partial pressure and pathlength, \( p_iL \). When pathlength is held constant, a change in the total pressure results in a proportional change to the product of partial pressure and pathlength. It is therefore of interest to determine the influence of total pressure when the partial pressure-pathlength is held constant. To this end, an additional case was investigated for H2O with \( Y_{H_2O} = 0.1 \) and \( p = 0.1 \) atm. This combination yields the same value of \( p_iL \) as the \( Y_{H_2O} = 0.01, p = 1 \) atm case presented in Fig. 4.10. As can be seen in Fig. 4.10a, this scenario resulted in a slightly different trend than the atmospheric case, with deviations in the two total pressure cases principally at low temperature. This demonstrates the modest influence of total pressure on emissivity for constant partial pressure-pathlength.
4.4 Radiative Transfer

4.4.1 Radiative Transfer at Variable Pressure

The impact of variable total pressure is now investigated through select predictions of radiative transfer in a one-dimensional layer of gas. Simulations were performed in which a layer of gas is bounded by walls at $T_w = 0$ K and zero reflectivity, in other words, the medium is bounded by vacuum. An analytical solution to the radiative transfer equation for an isothermal homogeneous gas layer was obtained, and the exact solutions for spectral radiative flux, $q_\eta$, and the radiative flux divergence, $-dq_\eta/dx$ are given by Eqs. (4-5) and (4-6).

$$q_\eta(x) = 2\pi I_{bn}(T) \left[ E_3 \left( \kappa_\eta(L - x) \right) - E_3 \left( \kappa_\eta x \right) \right]$$

(4-5)

$$-\frac{dq_\eta}{dx}(x) = -2\pi \kappa_\eta I_{bn}(T) \left[ E_2 \left( \kappa_\eta(L - x) \right) + E_2 \left( \kappa_\eta x \right) \right]$$

(4-6)

$I_{bn}$ is the Planck blackbody spectral intensity at the local temperature, and $E_2$ and $E_3$ are the exponential integral functions of the second and third order, respectively. To integrate, these equations are solved within each wavenumber interval, multiplied by the width of the wavenumber interval (in cm$^{-1}$), and summed, resulting in total radiative quantities. The same interval size and range was used as for all previous calculations.

Results from the spectral integration of Eqs. (4-5) and (4-6) are shown in Fig. 4.11 for a) CO$_2$, and b) H$_2$O at 1000 K. The left panels show total net radiative flux, and the right panels show the divergence of the net radiative flux. For the results shown in Fig. 4.11 the layer length was constant at 1 m, the mole fraction of H$_2$O or CO$_2$ was 0.3 (with air), and total pressure varied from 0.1 atm to 50 atm.
As seen in Fig. 4.11, an increase in total pressure generally leads to an increase in magnitude of both radiative flux and net radiative flux divergence. For CO₂ (Fig. 4.11a) it is seen that changes in total pressure have a strong impact, even at high pressure. This holds true at 2500 K as well. However, the results for H₂O show that changes in total pressure at higher pressure produce a relatively small change in the resulting radiative transfer within the gas layer. This is likely because the total emissivity (see Fig 4.10a) is increasing to the point that the layer is losing transparency (becoming optically thick) and thus approaches the case of emission from a solid at the prescribed gas temperature. Hence, a reduction of radiative flux within the layer is seen corresponding to a sharp increase in radiative flux near the walls. The changes in radiative transfer at the wall are always strongly impacted by total pressure increases over the pressures explored, and it is seen that exiting flux displays a significant increase with increasing total pressure. For H₂O, the impact of a pressure change at high pressure is slightly more pronounced at 2500 K due to the reduction in total emissivity seen in Fig. 4.10a, although the 8 atm solution remains close to the 50 atm solution within the gas layer. Because CO exhibits behavior similar to CO₂, it follows similar trends, and is therefore not illustrated here.

The results of Fig. 4.11 are for constant layer length with increasing total pressure. As pressure increases for constant layer length, the amount of radiating material increases. In order to examine only the effects of variable total pressure on property changes, the radiative transfer equation was again solved but with the mass held constant. At atmospheric pressure the layer length was set to 1 m, and the ideal gas law was used to calculate the layer length for varying pressure assuming constant mass. At the temperatures and pressures in question the ideal gas law is an excellent approximation for the species considered here.
Figure 4.11: Total net radiative flux (left graph), \( q \), and net radiative flux divergence (right graph), \(-\frac{dq}{dx}\), as a function of position, \( x \), for a) CO\(_2\) and b) H\(_2\)O at 1000 K and \( Y_i = 0.3 \). Results are shown for four total pressures varying from 0.1 atm to 50 atm.

The RTE was solved as described in the foregoing paragraph for the one-dimensional constant mass layer, again with \( Y_i = 0.3 \) and \( T_i = 1000 \) K and 2500 K. The results for the total net radiative flux exiting the gas layer for the scenarios investigated are shown as a function of total pressure in Fig. 4.12 for H\(_2\)O, CO\(_2\), and CO at a) 1000 K, and b) 2500 K. Note the change in
scale for the two panels. The layer length for the scenarios tested varied from 10 m (0.1 atm case) to 0.02 m (50 atm case). It can be seen that the exiting flux for the constant mass case increases as total pressure increases for all three species, and that most of this change occurs at low total pressure. Although the increase in exiting flux doesn’t change as total pressure increases by as much as was observed for the constant layer length scenario, the change is still quite significant. Increasing the pressure from 0.1 atm to 50 atm results in an increase in the exiting radiative flux by at most a factor of 2.2 for H$_2$O, 1.7 for CO$_2$, and 4.7 for CO at the temperatures investigated. The case of CO$_2$ at 2500 K (Fig. 4.12b) showed the least change over the pressure change considered, increasing by only 9.2%. The relatively large increase in exiting flux with pressure for CO suggests that neglecting the impact of CO in calculations, as is commonly done, may lead to non-negligible error at high pressure.

Figure 4.12: The predicted exiting total net radiative flux, $q_e$, for the three gas species investigated at a) 1000 K, and b) 2500 K.
4.4.2 Comparisons with Previous Work

Similar to the comparison of ALBDF data in Section 4.1.4, it is of interest to explore how the updated spectral data affect calculations of radiative transfer relative to predictions based on the ALBDF generated using previously generated absorption spectra. The line-by-line results for divergence of radiative flux from Denison (1994) are compared with the solution found using HITEMP 2010 as the source for spectral data. The discrete ordinates method, described previously (Solovjov and Webb, 2000), was applied for the present line-by-line calculations. A spatial grid of 200 points was used to discretize the space variable, and 36 ordinates were used in angular discretization. Iterations were suspended when the intensities ceased to change by more than $10^{-16}$ W/m$^2$ sr.

The choice of 36 ordinates came after a study showed it to be a good compromise between accuracy and computation time. For this study, a gray medium at 700 K with an absorption coefficient of 1 m$^{-1}$ was bounded by gray walls 1 m apart at 1200 K and 500 K with emissivities of 0.2 and 0.6. For the case of gray media, an exact analytical solution is possible. Figure 4.13 shows the error in the discrete ordinates method as compared to the exact analytical solution as a function of $n$, the number of ordinate directions. As can be seen, the error steadily decreases until about $n = 36$ at which point an increase in the number of ordinates does not further reduce the error in the discrete ordinates solution significantly. For more demanding computations, 36 ordinates is not a feasible choice, but for simple 1D cases, it is not unreasonable to use such fine resolution.
Figure 4.13: The average relative error in the discrete ordinates solution as compared to the exact analytical solution as a function of the number of ordinate directions, \( n \), for radiative flux and the divergence of the radiative flux.

The first case comparing line-by-line data is for a medium of 20% H\(_2\)O (remainder air) at 1500 K between black walls that are at 0 K and are 2 m apart. The solution for the divergence of radiative flux is seen in Fig. 4.14 using the HITEMP 2010 database and those reported by Denison (1994). As can be seen, there is a significant difference between the solutions. At the midpoint, the results from Denison differ by 21% relative to the results obtained using the HITEMP 2010 database. The error remains large nearer the walls.

The next case is for a medium of 30% CO\(_2\) at 1300 K between gray walls (\( \varepsilon = 0.9 \)) that are at 500 K and are spaced 5 m apart. The solution for the divergence of radiative flux is seen in Fig. 4.15 calculated using the HITEMP 2010 database and from Denison (1994). When the participating gas is CO\(_2\), the difference appears to be much smaller than for the case of H\(_2\)O, although the error is as high as 20% at the midpoint compared to the results obtained using HITEMP 2010. Overall, the agreement is better than that observed for H\(_2\)O in Fig. 4.14. In
general, previous calculations have been found to be very similar to calculations employing the HITEMP 2010 database when temperatures are about 1000 K or below. Above this value, the error increases due to the exclusion by previous databases of spectral lines that are only significant at elevated temperature.

Figure 4.14: The divergence of radiative flux, \(-dq/dx\), as a function of position. The medium is at \(p = 1\) atm, \(T = 1500\) K, and \(Y_{H_2O} = 0.2\). The walls are 2 m apart, and are black at 0 K.

Figure 4.15: The divergence of radiative flux, \(-dq/dx\), as a function of position. The medium is at \(p = 1\) atm, \(T = 1300\) K, and \(Y_{CO_2} = 0.3\). The walls are 5 m apart, and are at 500 K with an emissivity of 0.9.
4.5 Summary

ALBDF data for H₂O, CO₂, and CO were generated and presented, showing a shift in the ALBDF to lower values of \( F \) as total pressure increased. This shift was observed to be weaker at high temperature. Further, the previously documented shift due to increase in mole fraction of the species of interest was similar to that observed at atmospheric pressure and at high pressure. Finally, the ALBDF was shown to become less smooth as total pressure increases.

Total emissivity generated for the three species from the line-by-line absorption spectrum was presented for variable total pressure, and it was observed that pressure changes alone account for a significant change in emissivity, and a modest change when partial pressure-pathlength is held constant.

Total radiative flux and radiative flux divergence were calculated for a one-dimensional, isothermal layer for constant length and constant mass cases, revealing that total pressure changes result in a significant impact on radiative transfer. It can be concluded that total pressure changes alone can have a significant impact on radiative transfer in high temperature gaseous media. At a layer temperature of 1000 K the flux exiting a radiating gas layer of fixed mass exhibits a greater than four-fold increase with an increase in pressure from 0.1 to 50 atm as a result solely of associated changes in radiative property of the layer medium. The relative increase in exiting radiative flux is significantly lower for a layer temperature of 2500 K, except for CO. Therefore, the change in the ALBDF for variable total pressure can also be considered of significant importance, with diminishing relative influence at increasing temperature for H₂O and CO₂.

Comparisons were made with previous work for the ALBDF and for radiative transfer. These comparisons showed a substantial difference between the new results and the results of...
Denison (1994). This difference is smaller for CO₂, although it is still significant. It can be concluded that the previous correlations of the ALBDF (Denison and Webb, 1993b; Denison and Webb, 1995a), while accurate at nominal temperatures, benefited from the update permitted by the availability of the expanded HITEMP 2010 database.
In order for application of the SLW model to be feasible, the absorption line blackbody distribution function (ALBDF) must be implemented in an efficient manner. It has been established that the correlations of Denison and Webb (1993b, 1995a) are outdated and need to be updated and/or replaced. One of the primary contributions of this work is to provide efficient representations of the ALBDF that include improvements over previous representations.

The hyperbolic tangent correlation of the ALBDF has been widely adopted, and because of this it is desirable to retain this form in the update. Myriad other mathematical representations of the ALBDF are undoubtedly possible, but an exhaustive study of possibilities will not be conducted here. The retention of the hyperbolic tangent correlation will allow for more convenient implementation for users desiring to utilize the new version. The update and expansion of the hyperbolic tangent correlation will be presented first, followed by a discussion of using tabulated data directly. Finally, a third representation based on orthogonal polynomials will be presented. Following the presentation of these different representations of the ALBDF, a comparison will be made between line-by-line ABLDF data and the ALBDF representations. Lastly, computation time for use of the three methods will be considered.
5.1 Hyperbolic Tangent Correlation

As stated previously, the hyperbolic tangent correlation form of the ALBDF originally proposed by Denison and Webb (1993b) has been widely adopted. Because of this, this form will be the focus of the present update. While other correlation forms are possible, it seems prudent to use the form that is currently in use. Important improvements that have been made to this correlation form in this study include use of the updated and improved HITRAN 2010 spectroscopic database, more rigorous generation of the absorption cross-section data, extension of the temperature ceiling from 2500 K to 3000 K, extension the correlation to variable pressure, and correlation of the ALBDF of carbon monoxide.

5.1.1 Correlation at Atmospheric Pressure

The approach used in extending the ALBDF correlation is to prepare a correlation accurate at atmospheric pressure, then correct the atmospheric-pressure correlation for changes in total pressure. Thus, the first step in expanding the ALBDF to variable pressure is to prepare the correlation at atmospheric pressure. After line-by-line ALBDF data are generated, the correlation parameters are obtained by performing a least-squares curve fit to the data. The correlation for atmospheric pressure is of the form (Denison and Webb, 1993b)

\[
F(C, T_g, T_b, Y) = \frac{1}{2} \tanh[P(C, T_g, T_b, Y)] + \frac{1}{2},
\]

and

\[
P(C, T_g, T_b, Y = 0) = \sum_{i=0}^{3} \sum_{m=0}^{3} \sum_{n=0}^{3} b_{lmn} \left( \frac{T_g}{2500} \right)^n \left( \frac{T_b}{2500} \right)^m \xi^l,
\]

where \( \xi = \ln(C) \). The temperatures \( T_g \) and \( T_b \) are in K. As used in the ALBDF, it is more convenient to represent \( C \) in the units m\(^2\)/mol. These units are obtained by multiplying the absorption cross-section obtained in Section 4.1 by Avogadro's number and by converting cm to
Calculation of the absorption coefficient as shown in Eq. (3-3) is adjusted slightly in that the molar density \(N(p, T)\) no longer includes Avogadro's number since it is applied through \(C\). The set of 64 coefficients \(b_{lmn}\) has been obtained for H\(_2\)O, CO\(_2\), and CO for atmospheric pressure using the HIT\(\)EMP 2010 database, and these can be found in Table 5-1. The data utilized in the least-squares fit were generated at combinations of \(T_g\) and \(T_b\) ranging from 400 K to 3000 K, spaced every 200 K.

<table>
<thead>
<tr>
<th>((l,m,n))</th>
<th>(b_{lmn})</th>
<th>(c_{lmn})</th>
<th>(CO_2)</th>
<th>(CO)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0)</td>
<td>0.978924</td>
<td>1.68529</td>
<td>1.83492</td>
<td>3.31631</td>
</tr>
<tr>
<td>(0,0,1)</td>
<td>-0.207426</td>
<td>-2.91926</td>
<td>-1.82218</td>
<td>0.273254</td>
</tr>
<tr>
<td>(0,0,2)</td>
<td>-2.80673</td>
<td>1.41928</td>
<td>1.27833</td>
<td>-1.03538</td>
</tr>
<tr>
<td>(0,0,3)</td>
<td>1.38942</td>
<td>-0.209800</td>
<td>-1.03538</td>
<td>0.473980</td>
</tr>
<tr>
<td>(0,1,0)</td>
<td>2.43339</td>
<td>0.160822</td>
<td>-1.54969</td>
<td>-7.97411</td>
</tr>
<tr>
<td>(0,1,1)</td>
<td>-5.54212</td>
<td>-5.18188</td>
<td>1.11312</td>
<td>0.546750</td>
</tr>
<tr>
<td>(0,1,2)</td>
<td>16.9379</td>
<td>4.53813</td>
<td>-2.42581</td>
<td>1.63988</td>
</tr>
<tr>
<td>(0,1,3)</td>
<td>-7.31920</td>
<td>0.919086</td>
<td>-0.875344</td>
<td>0.687532</td>
</tr>
<tr>
<td>(0,2,0)</td>
<td>-2.27043</td>
<td>0.593801</td>
<td>3.51788</td>
<td>15.3245</td>
</tr>
<tr>
<td>(0,2,1)</td>
<td>9.80203</td>
<td>-2.66943</td>
<td>-1.14955</td>
<td>-3.64425</td>
</tr>
<tr>
<td>(0,2,2)</td>
<td>-24.4373</td>
<td>2.02036</td>
<td>3.54657</td>
<td>-0.372778</td>
</tr>
<tr>
<td>(0,2,3)</td>
<td>10.2661</td>
<td>-1.51642</td>
<td>0.919086</td>
<td>-0.875344</td>
</tr>
<tr>
<td>(0,3,0)</td>
<td>0.968416</td>
<td>0.0616066</td>
<td>-1.50580</td>
<td>-7.96232</td>
</tr>
<tr>
<td>(0,3,1)</td>
<td>-4.41664</td>
<td>-0.227721</td>
<td>0.522032</td>
<td>3.98204</td>
</tr>
<tr>
<td>(0,3,2)</td>
<td>10.2661</td>
<td>0.166014</td>
<td>-1.65400</td>
<td>-2.02479</td>
</tr>
<tr>
<td>(0,3,3)</td>
<td>-4.20383</td>
<td>0.729684</td>
<td>0.457744</td>
<td>0.687532</td>
</tr>
<tr>
<td>(1,0,0)</td>
<td>0.231177</td>
<td>-1.19664</td>
<td>0.202157</td>
<td>0.427225</td>
</tr>
<tr>
<td>(1,0,1)</td>
<td>-0.0946050</td>
<td>3.13626</td>
<td>0.885000</td>
<td>0.159348</td>
</tr>
<tr>
<td>(1,0,2)</td>
<td>0.908440</td>
<td>-1.97238</td>
<td>-0.982475</td>
<td>-0.314632</td>
</tr>
<tr>
<td>(1,0,3)</td>
<td>-0.538832</td>
<td>-0.538832</td>
<td>0.375315</td>
<td>0.152077</td>
</tr>
<tr>
<td>(1,1,0)</td>
<td>0.253813</td>
<td>-1.47806</td>
<td>-0.531916</td>
<td>-1.35629</td>
</tr>
<tr>
<td>(1,1,1)</td>
<td>2.08204</td>
<td>17.7436</td>
<td>-2.21448</td>
<td>0.115369</td>
</tr>
<tr>
<td>(1,1,2)</td>
<td>-4.47671</td>
<td>-15.5388</td>
<td>2.29322</td>
<td>0.658528</td>
</tr>
<tr>
<td>(1,1,3)</td>
<td>2.44379</td>
<td>-0.867072</td>
<td>-0.372593</td>
<td>3.66386</td>
</tr>
<tr>
<td>(1,2,0)</td>
<td>-0.337419</td>
<td>-2.40775</td>
<td>1.01979</td>
<td>3.66386</td>
</tr>
</tbody>
</table>

Table 5-1: The correlation coefficients \(b_{lmn}\) for H\(_2\)O (left set of H\(_2\)O coefficients), CO\(_2\), and CO for Eq. (5-2). For H\(_2\)O, the coefficients \(c_{lmn}\) for Eq. (5-4) are also given (right set of H\(_2\)O coefficients).
<table>
<thead>
<tr>
<th>(l,m,n)</th>
<th>H₂O</th>
<th>CO₂</th>
<th>CO</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>b₁₅₅₅</td>
<td>c₁₅₅₅</td>
<td></td>
</tr>
<tr>
<td>(1,2,1)</td>
<td>-2.30864</td>
<td>9.54136</td>
<td>1.91290</td>
</tr>
<tr>
<td>(1,2,2)</td>
<td>4.63425</td>
<td>-7.05450</td>
<td>-1.68833</td>
</tr>
<tr>
<td>(1,2,3)</td>
<td>-2.47350</td>
<td>0.600486</td>
<td>0.0888357</td>
</tr>
<tr>
<td>(1,3,0)</td>
<td>0.179163</td>
<td>-0.247551</td>
<td>-0.506065</td>
</tr>
<tr>
<td>(1,3,1)</td>
<td>0.787972</td>
<td>0.835499</td>
<td>-0.526424</td>
</tr>
<tr>
<td>(1,3,2)</td>
<td>-1.52075</td>
<td>-0.589727</td>
<td>0.340073</td>
</tr>
<tr>
<td>(1,3,3)</td>
<td>0.829104</td>
<td>-0.101266</td>
<td>0.564327</td>
</tr>
<tr>
<td>(2,0,0)</td>
<td>0.166909</td>
<td>-0.156309</td>
<td>0.054472216</td>
</tr>
<tr>
<td>(2,0,1)</td>
<td>-0.795281</td>
<td>-1.63344</td>
<td>-0.158181</td>
</tr>
<tr>
<td>(2,0,2)</td>
<td>0.939269</td>
<td>1.49051</td>
<td>0.290036</td>
</tr>
<tr>
<td>(2,0,3)</td>
<td>-0.304703</td>
<td>0.538061</td>
<td>0.127097</td>
</tr>
<tr>
<td>(2,1,0)</td>
<td>-0.669061</td>
<td>2.15385</td>
<td>-0.172337</td>
</tr>
<tr>
<td>(2,1,1)</td>
<td>3.93941</td>
<td>-23.6019</td>
<td>0.538061</td>
</tr>
<tr>
<td>(2,1,2)</td>
<td>-4.43049</td>
<td>20.8035</td>
<td>-0.853519</td>
</tr>
<tr>
<td>(2,1,3)</td>
<td>1.19632</td>
<td>0.383656</td>
<td>0.0318698</td>
</tr>
<tr>
<td>(2,2,0)</td>
<td>0.837513</td>
<td>3.34190</td>
<td>0.233086</td>
</tr>
<tr>
<td>(2,2,1)</td>
<td>-0.304703</td>
<td>-0.137608</td>
<td>0.032405</td>
</tr>
<tr>
<td>(2,2,2)</td>
<td>0.939269</td>
<td>1.49051</td>
<td>0.290036</td>
</tr>
<tr>
<td>(2,2,3)</td>
<td>-0.976627</td>
<td>-0.458833</td>
<td>0.0318698</td>
</tr>
<tr>
<td>(2,3,0)</td>
<td>-0.321007</td>
<td>0.344856</td>
<td>-0.101433</td>
</tr>
<tr>
<td>(2,3,1)</td>
<td>1.90733</td>
<td>-1.14900</td>
<td>0.291151</td>
</tr>
<tr>
<td>(2,3,2)</td>
<td>-1.76314</td>
<td>0.807114</td>
<td>-0.424021</td>
</tr>
<tr>
<td>(2,3,3)</td>
<td>0.215567</td>
<td>0.184048</td>
<td>0.111101</td>
</tr>
<tr>
<td>(3,0,0)</td>
<td>0.0189884</td>
<td>0.408081</td>
<td>6.30156E-03</td>
</tr>
<tr>
<td>(3,0,1)</td>
<td>-0.0755879</td>
<td>0.218904</td>
<td>-0.0300971</td>
</tr>
<tr>
<td>(3,0,2)</td>
<td>0.0692804</td>
<td>-0.421655</td>
<td>0.0445779</td>
</tr>
<tr>
<td>(3,0,3)</td>
<td>2.47619E-06</td>
<td>-0.0194831</td>
<td>-8.80491E-04</td>
</tr>
<tr>
<td>(3,1,0)</td>
<td>-0.0794413</td>
<td>-0.988248</td>
<td>-0.0182273</td>
</tr>
<tr>
<td>(3,1,1)</td>
<td>0.346149</td>
<td>10.5424</td>
<td>0.0950925</td>
</tr>
<tr>
<td>(3,1,2)</td>
<td>-0.231489</td>
<td>-9.32335</td>
<td>-0.122626</td>
</tr>
<tr>
<td>(3,1,3)</td>
<td>-0.0657353</td>
<td>0.0501599</td>
<td>-5.01261E-03</td>
</tr>
<tr>
<td>(3,2,0)</td>
<td>0.0969300</td>
<td>-1.51699</td>
<td>0.0209971</td>
</tr>
<tr>
<td>(3,2,1)</td>
<td>-0.404604</td>
<td>5.85632</td>
<td>-0.109841</td>
</tr>
<tr>
<td>(3,2,2)</td>
<td>0.151771</td>
<td>-4.31687</td>
<td>0.134897</td>
</tr>
<tr>
<td>(3,2,3)</td>
<td>0.177646</td>
<td>-0.0540501</td>
<td>3.91750E-03</td>
</tr>
<tr>
<td>(3,3,0)</td>
<td>-0.0367609</td>
<td>-0.156857</td>
<td>-8.18055E-03</td>
</tr>
<tr>
<td>(3,3,1)</td>
<td>0.147107</td>
<td>0.520449</td>
<td>0.0416371</td>
</tr>
<tr>
<td>(3,3,2)</td>
<td>-0.0148638</td>
<td>-0.365078</td>
<td>-0.0502137</td>
</tr>
<tr>
<td>(3,3,3)</td>
<td>-0.0984692</td>
<td>0.0200237</td>
<td>6.06937E-03</td>
</tr>
</tbody>
</table>
For each combination of $T_g$ and $T_b$, the ALBDF was generated for a range of absorption cross-sections beginning at $C_{min} = 10^{-4}$ m$^2$/mol for all species and extending up to $C_{max} = 60$ m$^2$/mol for H$_2$O and CO and $C_{max} = 600$ m$^2$/mol for CO$_2$. The ALBDF asymptotes to unity when the absorption cross-section approaches these maximum values. This occurs for higher values of absorption cross-section for CO$_2$ due to a particularly strong absorption band. It was found that predictions of radiative transfer are negligibly impacted by the absorption cross-section range below $C_{min} = 10^{-4}$ m$^2$/mol. For example, when a lower bound of $10^{-4}$ m$^2$/mol is used for CO$_2$, the error compared to the much lower bound of $10^{-7}$ m$^2$/mol was found to be 0.25% or less for calculations of radiative transfer, total emissivity, or Planck-mean absorption coefficient. Similar error would be expected for CO, and less error is expected for H$_2$O since frequently the ALBDF has a value at or near zero at the lower bound of $10^{-4}$ m$^2$/mol.

The ALBDF data are logarithmically spaced at 100 points between the minimum and maximum value of $C$. For most of these sets of ALBDF data, there is a series of consecutive values of $C$ where $F$ is constant at either 0 or 1 at the extremes. Because of the mathematical difficulties inherent in fitting a curve to a straight horizontal line, these portions of ALBDF data, if included in the least-squares fit, were found to reduce the accuracy of the correlation and were therefore excluded. This was done by removing ALBDF data in the generation of the least-squares correlation nearly equal to 0 and 1. An optimization was performed, and data were removed from the least-squares curve fit that fell within 0.01 of either 0 or 1 for H$_2$O, 0.007 for CO$_2$, and 0.005 for CO. Changing the threshold for excluding ALBDF data near 0 and 1 from these values increased the error when comparing the correlation to the LBL data for CO$_2$ and CO. For H$_2$O, the error continues to decrease as the threshold is increased from 0.01, but it was found that the overall stability of the correlation deteriorates if the threshold is too high, so a
value of 0.01 was chosen as a compromise. Removing these data near 0 and 1 from the curve fit was found to increase the accuracy of the correlation even within the regions of C where the ALBDF data were excluded from the curve fit.

Although the bounds of C for which the correlation was designed (i.e., \( C_{\text{min}} \) and \( C_{\text{max}} \)) are those stated above, it was found that the correlations for \( \text{H}_2\text{O} \) and \( \text{CO}_2 \) are quite well-behaved and can be extended beyond these absorption cross-section bounds safely, up to at least a few orders of magnitude at either extreme. However, CO exhibits more irregular behavior, and its correlation should only be used within the absorption cross-section bounds specified.

As shown previously, the ALBDF for \( \text{H}_2\text{O} \) displays rather significant dependence on mole fraction. The atmospheric-pressure ALBDF correlation for \( \text{H}_2\text{O} \) can be expanded to allow for variable mole fraction by replacing \( \xi \) in Eq. (5-2) with \( \xi - \xi_{sb} \) as seen below (Denison and Webb, 1993b).

\[
P(C,T_g,T_b,Y) = \sum_{i=0}^{3} \sum_{m=0}^{3} \sum_{n=0}^{3} b_{lmn} \left( \frac{T_g}{2500} \right)^n \left( \frac{T_b}{2500} \right)^m (\xi - \xi_{sb})^i, \tag{5-3}
\]

where

\[
\xi_{sb} = \sum_{i=0}^{3} \sum_{m=0}^{3} \sum_{n=0}^{2} c_{lmn} \left( \frac{T_b}{2500} \right)^n \xi^m Y^{i+1}. \tag{5-4}
\]

The empirical coefficients \( c_{lmn} \) can be found in Table 5.1. They were found using a least-squares fit to line-by-line data generated for \( \text{H}_2\text{O} \) mole fractions of approaching 0 and equal to 0.05, 0.1, 0.2, 0.3, 0.4, 0.6, 0.8, and 1.0. This was done by first obtaining the line-by-line ALBDF for each temperature combination. These ALBDF data were used to obtain \( P(C,T_g,T_b,Y) \) according to Eq. (5-1), and then Eq. (5-3) was solved implicitly for \( \xi_{sb} \). This parameter is used in the least-squares fit according to Eq. (5-4) to solve for \( c_{lmn} \). Finer resolution of the ALBDF was used at low mole fraction because the ALBDF is more sensitive to mole fraction changes in this range. The data
employed in this curve fit were subject to the same temperature and absorption cross-section ranges specified previously. As documented previously in Sections 4.1.2 and 4.1.3, for CO₂ and CO, a careful investigation revealed that the influence of mole fraction can be safely neglected for the purposes of the ALBDF. Consequently, there is no need to correlate the behavior for these species as a function of mole fraction.

5.1.2 Variable Pressure Correction

The dependence of the ALBDF on total pressure is similar to the dependence of the ALBDF for H₂O on mole fraction. Thus, the total pressure dependence in the correlation is included in much the same way that variable mole fraction is included for the ALBDF correlation of H₂O. A simple shift from the correlation for atmospheric pressure is used. For H₂O and CO₂, \( \xi \) in Eq. (5-2) is replaced with \( \xi - \xi_p \) (Denison and Webb, 1996a), where

\[
\xi_p = \sum_{l=0}^{3} \sum_{m=0}^{3} \sum_{n=0}^{3} d_{lmn} \left( \frac{T_g T_b}{2500^2} \right)^n \xi^m \psi^{l+1},
\]

and

\[
\psi = \ln(100 p_e)/10.
\]

The coefficients \( d_{lmn} \) are found in Table 5-2 and were obtained using a least-squares fit to the ALBDF generated from line-by-line data. The total pressure range for which this correlation is valid is 0.1 atm to 50 atm, and ALBDF data generated at pressures of 0.1, 0.25, 0.5, 1, 2, 4, 8, 15, 30, and 50 atm were used in the least-squares fit. Similar to the mole fraction dependence of H₂O, it was found that the ALBDF is more sensitive to total pressure changes at low pressure. For this reason, the resolution in total pressure employed at low pressure is finer than at high pressure.
Table 5-2: The coefficients $d_{lmn}$ used in Eq. (5-5) for H$_2$O and CO$_2$ and Eq. (5-10) for CO.

<table>
<thead>
<tr>
<th>$(l,m,n)$</th>
<th>H$_2$O</th>
<th>CO$_2$</th>
<th>CO</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0)</td>
<td>-15.032</td>
<td>-14.9838</td>
<td>-7.98027</td>
</tr>
<tr>
<td>(0,0,1)</td>
<td>41.160</td>
<td>38.4168</td>
<td>12.4484</td>
</tr>
<tr>
<td>(0,0,2)</td>
<td>-44.062</td>
<td>-37.0871</td>
<td>-13.1125</td>
</tr>
<tr>
<td>(0,0,3)</td>
<td>15.958</td>
<td>11.6340</td>
<td>4.86872</td>
</tr>
<tr>
<td>(0,1,0)</td>
<td>2.8319</td>
<td>-0.279677</td>
<td>-1.02985</td>
</tr>
<tr>
<td>(0,1,1)</td>
<td>-1.4503</td>
<td>-2.38649</td>
<td>5.34306</td>
</tr>
<tr>
<td>(0,1,2)</td>
<td>4.1039</td>
<td>3.48832</td>
<td>-4.23212</td>
</tr>
<tr>
<td>(0,1,3)</td>
<td>-2.7305</td>
<td>-1.65531</td>
<td>1.06388</td>
</tr>
<tr>
<td>(0,2,0)</td>
<td>-0.17598</td>
<td>0.240326</td>
<td>-0.125523</td>
</tr>
<tr>
<td>(0,2,1)</td>
<td>2.0712</td>
<td>-1.25365</td>
<td>0.290173</td>
</tr>
<tr>
<td>(0,2,2)</td>
<td>-0.95861</td>
<td>0.926603</td>
<td>0.608825</td>
</tr>
<tr>
<td>(0,2,3)</td>
<td>-0.16164</td>
<td>-0.175742</td>
<td>-0.457269</td>
</tr>
<tr>
<td>(0,3,0)</td>
<td>-0.080753</td>
<td>0.0268384</td>
<td>-0.0106483</td>
</tr>
<tr>
<td>(0,3,1)</td>
<td>0.42606</td>
<td>-0.0747372</td>
<td>-8.65797E-03</td>
</tr>
<tr>
<td>(0,3,2)</td>
<td>-0.41713</td>
<td>0.0107825</td>
<td>0.0960110</td>
</tr>
<tr>
<td>(0,3,3)</td>
<td>0.12426</td>
<td>0.0200397</td>
<td>-0.0561090</td>
</tr>
<tr>
<td>(1,0,0)</td>
<td>51.460</td>
<td>65.6646</td>
<td>30.9290</td>
</tr>
<tr>
<td>(1,0,1)</td>
<td>-129.85</td>
<td>-153.130</td>
<td>-62.5849</td>
</tr>
<tr>
<td>(1,0,2)</td>
<td>128.98</td>
<td>134.518</td>
<td>76.9683</td>
</tr>
<tr>
<td>(1,0,3)</td>
<td>-43.877</td>
<td>-38.4988</td>
<td>-30.9382</td>
</tr>
<tr>
<td>(1,1,0)</td>
<td>-10.451</td>
<td>3.73194</td>
<td>7.65692</td>
</tr>
<tr>
<td>(1,1,1)</td>
<td>11.362</td>
<td>-6.34557</td>
<td>-28.7984</td>
</tr>
<tr>
<td>(1,1,2)</td>
<td>-31.935</td>
<td>4.11347</td>
<td>26.6729</td>
</tr>
<tr>
<td>(1,1,3)</td>
<td>19.613</td>
<td>0.442688</td>
<td>-8.60570</td>
</tr>
<tr>
<td>(1,2,0)</td>
<td>2.4344</td>
<td>-1.45712</td>
<td>2.10411</td>
</tr>
<tr>
<td>(1,2,1)</td>
<td>-13.240</td>
<td>4.49358</td>
<td>-2.63598</td>
</tr>
<tr>
<td>(1,2,2)</td>
<td>7.4855</td>
<td>-1.90407</td>
<td>-1.77788</td>
</tr>
<tr>
<td>(1,2,3)</td>
<td>0.030561</td>
<td>-0.230432</td>
<td>1.65135</td>
</tr>
<tr>
<td>(1,3,0)</td>
<td>0.56745</td>
<td>-0.194709</td>
<td>0.177021</td>
</tr>
<tr>
<td>(1,3,1)</td>
<td>-2.6102</td>
<td>0.344715</td>
<td>-0.0559326</td>
</tr>
<tr>
<td>(1,3,2)</td>
<td>2.6208</td>
<td>0.0823013</td>
<td>-0.401553</td>
</tr>
<tr>
<td>(1,3,3)</td>
<td>-0.80700</td>
<td>-0.169292</td>
<td>0.245225</td>
</tr>
<tr>
<td>(2,0,0)</td>
<td>-49.884</td>
<td>-90.4978</td>
<td>-34.7347</td>
</tr>
<tr>
<td>(2,0,1)</td>
<td>105.44</td>
<td>191.277</td>
<td>103.848</td>
</tr>
</tbody>
</table>
Table 5-2 Continued.

<table>
<thead>
<tr>
<th>((l,m,n))</th>
<th>(\text{H}_2\text{O})</th>
<th>(\text{CO}_2)</th>
<th>(\text{CO})</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2,0,2)</td>
<td>-85.162</td>
<td>-145.302</td>
<td>-141.729</td>
</tr>
<tr>
<td>(2,0,3)</td>
<td>22.810</td>
<td>34.0182</td>
<td>58.4544</td>
</tr>
<tr>
<td>(2,1,0)</td>
<td>11.367</td>
<td>-10.4392</td>
<td>-15.4238</td>
</tr>
<tr>
<td>(2,1,1)</td>
<td>-24.248</td>
<td>40.1084</td>
<td>49.4731</td>
</tr>
<tr>
<td>(2,1,2)</td>
<td>66.901</td>
<td>-43.2913</td>
<td>-48.5774</td>
</tr>
<tr>
<td>(2,1,3)</td>
<td>-39.492</td>
<td>12.8299</td>
<td>16.9208</td>
</tr>
<tr>
<td>(2,2,0)</td>
<td>-5.9424</td>
<td>2.55105</td>
<td>-5.54724</td>
</tr>
<tr>
<td>(2,2,1)</td>
<td>24.356</td>
<td>-6.77085</td>
<td>5.73240</td>
</tr>
<tr>
<td>(2,2,2)</td>
<td>-14.925</td>
<td>2.07528</td>
<td>1.98725</td>
</tr>
<tr>
<td>(2,2,3)</td>
<td>0.80233</td>
<td>0.815010</td>
<td>-2.23242</td>
</tr>
<tr>
<td>(2,3,0)</td>
<td>-1.0839</td>
<td>0.400183</td>
<td>-0.466208</td>
</tr>
<tr>
<td>(2,3,1)</td>
<td>4.5969</td>
<td>-0.766811</td>
<td>0.190251</td>
</tr>
<tr>
<td>(2,3,2)</td>
<td>-4.6497</td>
<td>0.0184473</td>
<td>0.635514</td>
</tr>
<tr>
<td>(2,3,3)</td>
<td>1.4447</td>
<td>0.238835</td>
<td>-0.389172</td>
</tr>
<tr>
<td>(3,0,0)</td>
<td>14.967</td>
<td>41.9412</td>
<td>11.6182</td>
</tr>
<tr>
<td>(3,0,1)</td>
<td>-21.834</td>
<td>-79.9944</td>
<td>-57.7850</td>
</tr>
<tr>
<td>(3,0,2)</td>
<td>6.4337</td>
<td>49.6038</td>
<td>84.5068</td>
</tr>
<tr>
<td>(3,0,3)</td>
<td>2.4764</td>
<td>-7.29429</td>
<td>-35.1080</td>
</tr>
<tr>
<td>(3,1,0)</td>
<td>-4.1549</td>
<td>7.51407</td>
<td>8.76613</td>
</tr>
<tr>
<td>(3,1,1)</td>
<td>14.831</td>
<td>-36.3335</td>
<td>-27.3782</td>
</tr>
<tr>
<td>(3,1,2)</td>
<td>-39.792</td>
<td>42.5186</td>
<td>28.3922</td>
</tr>
<tr>
<td>(3,1,3)</td>
<td>22.768</td>
<td>-14.3027</td>
<td>-10.3480</td>
</tr>
<tr>
<td>(3,2,0)</td>
<td>3.6337</td>
<td>-1.43154</td>
<td>3.65583</td>
</tr>
<tr>
<td>(3,2,1)</td>
<td>-13.111</td>
<td>4.09735</td>
<td>-3.37356</td>
</tr>
<tr>
<td>(3,2,2)</td>
<td>8.1435</td>
<td>-1.86436</td>
<td>-0.873747</td>
</tr>
<tr>
<td>(3,2,3)</td>
<td>-0.57270</td>
<td>-0.109474</td>
<td>1.05051</td>
</tr>
<tr>
<td>(3,3,0)</td>
<td>0.57955</td>
<td>-0.256916</td>
<td>0.305052</td>
</tr>
<tr>
<td>(3,3,1)</td>
<td>-2.3468</td>
<td>0.610041</td>
<td>-0.0945290</td>
</tr>
<tr>
<td>(3,3,2)</td>
<td>2.3494</td>
<td>-0.249699</td>
<td>-0.378667</td>
</tr>
<tr>
<td>(3,3,3)</td>
<td>-0.72409</td>
<td>-0.0383282</td>
<td>0.219050</td>
</tr>
</tbody>
</table>

In Eq. (5-6), \(p_e\) is the equivalent pressure (Ludwig et al., 1973), and is defined as

\[
p_e = [1 + (B - 1)Y]p,
\]

(5-7)

\[
B = \frac{\gamma_{self}}{\gamma_{air}},
\]

(5-8)
where $B$ is the self-broadening coefficient. The value of $B$ was calculated at each temperature by averaging the ratio of half-width from self-broadening, $\gamma_{\text{self}}$, to half-width from air-broadening, $\gamma_{\text{air}}$, for all significant lines. These calculations were made for H$_2$O, CO$_2$, and CO over the temperature range investigated in this study, and results are displayed in Fig. 5.1. Further justification is seen in the figure for neglecting self-broadening effects, since the effect of air- and self-broadening is very similar for CO$_2$ and CO, indicated by $B$ values near unity. Because the effect of self-broadening for CO$_2$ and CO can be neglected, the equivalent pressure reduces to $p_e = p$. For H$_2$O, it can be seen that self-broadening has a significantly different impact than air-broadening. The average value of $B = 9.17$ was calculated to represent the full temperature range. It was found that including a temperature dependence as was done previously (Denison and Webb, 1996a) does not significantly improve results. The equivalent pressure for H$_2$O based on this investigation is $p_e = (1 + 8.17Y)p$.

![Figure 5.1: The ratio of self- to air-broadening, $B$, as a function of temperature for H$_2$O, CO$_2$, and CO.](image)
It was found that including the total pressure dependence for CO using the same approach as was used for H2O and CO2 resulted in unacceptable accuracy. This is because the term $\xi - \xi_p$ can be considered to be a shift in absorption cross-section (horizontal shift in the $F$ versus $C$ plot) from the correlation for ALBDF. This works well for the correlations for H2O and CO2 where the ALBDF correlation always decreases until it reaches zero as absorption cross-section is reduced. The atmospheric correlation for CO, on the other hand, is less well-behaved and does not follow this behavior. For this reason, the correlation for CO is shifted with ALBDF (vertical shift in the $F$ versus $C$ plot), with the shift being applied as follows:

$$F(C, T_g, T_b, p) = \frac{1}{2} \tanh\left[p(C, T_g, T_b, Y = 0) - P_p\right] + \frac{1}{2},$$

(5-9)

where

$$P_p = \sum_{l=0}^{3} \sum_{m=0}^{3} \sum_{n=0}^{3} d_{lmn} \left(\frac{T_g T_b}{2500^2}\right)^n \times \psi^{l+1}.$$  

(5-10)

It can be seen that the pressure-dependent term is identical to the one used for H2O and CO2, and the coefficients $d_{lmn}$ were obtained in the same manner with the same restrictions.

5.2 Tabulated Data

Computational capabilities have progressed to the point that representing the ALBDF using tabulated line-by-line data (a “look-up table” approach) is now a viable option. As part of this study, tabulated line-by-line ALBDF data for H2O, CO2, and CO have been made available on the website http://albdf.byu.edu. The tables contain data for 28 values of $T_g$ and $T_b$ ranging from 300 to 3000 K at 100 K intervals, for 71 values of absorption cross-section logarithmically spaced from $1e-4$ to $1000 \text{m}^2/\text{mol}$ (10 increments per decade), and for the 10 total pressures (0.1,
0.25, 0.5, 1, 2, 4, 8, 15, 30, and 50 atm) and nine H₂O mole fractions (0, 0.05, 0.1, 0.2, 0.3, 0.4, 0.6, 0.8, and 1.0) described previously for the least-squares fit.

It is expected that the tabulated ALBDF data will yield greater accuracy in practical computations than the hyperbolic tangent correlation of the ALBDF. However, there are attendant memory and data-read considerations. The relative accuracy of the tabulated data and correlation will be explored in some detail in a later section. When using the tabulated data in computations, there is an initial computational cost to read the data, after which only interpolation is required to obtain needed ALBDF values. The interpolation step requires significantly less CPU time than calculation of the hyperbolic tangent function requires for evaluation of the ALBDF. Thus, a solution in which the ALBDF is accessed a large number of times may be less computationally expensive if the tabulated data are used instead of the correlation. Computation time is discussed in greater detail in Section 5.6. For a single value of total pressure, the data in the table have an approximate size of 0.5 megabytes for CO₂ and CO and 5 megabytes for H₂O. The H₂O database is larger because it must include the data at all mole fractions. Because most combustion systems are at constant total pressure, at most the data for two pressures will need to be accessed, which will prevent the user from needing to read in the full set of data at all total pressures. It will be demonstrated hereafter that the resolution of the table is fine enough that a simple linear interpolation scheme yields line-by-line accuracy in the calculation of the ALBDF. The user could reduce the resolution or extent of the database and/or apply a different interpolation scheme as desired.

5.3 Orthogonal Polynomials

A third representation of the ALBDF was briefly explored, that of using orthogonal polynomials. Orthogonal polynomials give convenient flexibility to expand to higher order
representations and their orthogonality makes them a good choice for curve fitting. To apply this method, the absorption cross-section was represented by a number of orthogonal polynomials (Trefethen, 1997) and the orthogonal polynomials and other variables were then used in a simple curve fit to line-by-line data. This form was applied to the three species considered in this study at atmospheric pressure. The other parameter ranges (gas temperature, blackbody temperature, etc.) were identical to those used for the other representations of the ALBDF already discussed. The work described in this section is preliminary and is not recommended for use in its current state, but is documented here as it may hold promise for future study.

As mentioned, the absorption cross-section was represented by a set of orthogonal polynomials. These polynomials have the form

\[ O_P^n = \sum_{i=0}^{n} A_i C^i, \]  

(5-11)

where the current polynomial \( (O_P^n) \) is of order \( n \) with coefficients \( A_i \) on each of the terms. The set of orthogonal polynomials contains the polynomial of order \( n \) and all polynomials of smaller order. For example, a third order set of orthogonal polynomials contain the following polynomials:

\[ O_P^1 = A_0 + A_1 C, \]
\[ O_P^2 = A_2 + A_3 C + A_4 C^2, \]  
\[ O_P^3 = A_5 + A_6 C + A_7 C^2 + A_8 C^3. \]  

(5-12)

In this example, the coefficients \( A_i \) are numbered from 0 to 8 to illustrate that they each have a different value. The order of the set of polynomials can be increased to improve the accuracy of the curve fit.

After the orthogonal polynomials have been generated, a least-squares curve fit can be performed to generate empirical coefficients for the correlation of the ALBDF in the form
\[ \ln(F) = B_0 + B_1 T_g + B_2 T_b + B_3 Y + B_4 O\text{P}_1 + B_5 O\text{P}_2 + B_6 O\text{P}_3 + \cdots \]
\[ + B_7 T_g T_b + B_8 T_g Y + B_9 T_b Y + B_{10} T_g O\text{P}_1 + B_{11} T_g O\text{P}_2 + B_{12} T_g O\text{P}_3 + \cdots \]
\[ + B_{13} T_b O\text{P}_1 + B_{14} T_b O\text{P}_2 + B_{15} T_b O\text{P}_3 + \cdots \]
\[ + B_{16} Y O\text{P}_1 + B_{17} Y O\text{P}_2 + B_{18} Y O\text{P}_3 + \cdots \]
\[ + B_{19} T_g T_b Y + B_{20} T_g T_b O\text{P}_1 + B_{21} T_g T_b O\text{P}_2 + B_{22} T_g T_b O\text{P}_3 + \cdots \]
\[ + B_{23} T_g Y O\text{P}_1 + B_{24} T_g Y O\text{P}_2 + B_{25} T_g Y O\text{P}_3 + \cdots \]
\[ + B_{26} T_b Y O\text{P}_1 + B_{27} T_b Y O\text{P}_2 + B_{28} T_b Y O\text{P}_3 + \cdots \]
\[ + B_{29} T_g T_b Y O\text{P}_1 + B_{24} T_g T_b Y O\text{P}_2 + B_{25} T_g T_b Y O\text{P}_3 + \cdots . \]

Equation (5-13)

The coefficients, \( B_i \), were obtained in a preliminary investigation of this correlation form. The ellipses (\( \cdots \)) are noted in Eq. (5-13) to show where the correlation could be expanded to include higher order orthogonal polynomials. Further, Eq. (5-13) includes a mole fraction dependence as would be the case for the \( \text{H}_2\text{O} \) correlation. The terms that include \( Y \) are simply removed for \( \text{CO}_2 \) or \( \text{CO} \). If variable total pressure was included as a variable in the correlation, the effective pressure \( p_e \) would take the place of \( Y \) in Eq. (5-13).

As can be seen, Eqs. (5-12) and (5-13) rely only on multiplication and addition to compute \( F \). Not only does this make this correlation form simple and easy to implement, but it renders calculation of \( F \) significantly faster than the other representations of the ALBDF, as will be shown in the Section 5.6. However, the orthogonal polynomial correlation form as outlined in this preliminary exploration suffers from poor accuracy relative to the hyperbolic tangent correlation and the tabulated data, and thus, it was abandoned relative to the more accurate hyperbolic tangent correlation and tabulated data representations of the ALBDF. Thus, the results for the orthogonal polynomial are included here as having promise, but requiring significantly more development. Figure 5.2 shows the ALBDF as a function of absorption cross-section for a) \( \text{H}_2\text{O} \), and b) \( \text{CO}_2 \) at \( T_b = 1000 \) and various \( T_g \) as shown. Shown are line-by-line
(LBL) results and the orthogonal polynomial correlation (OP). The results are for atmospheric total pressure and the mole fraction of each species is in the limit of air-broadening only. As can be seen, the orthogonal polynomial form adopted is prone to oscillatory behavior and does not restrict the ALBDF to fall between 0 and 1 as the hyperbolic tangent form does. The orthogonal polynomial form has poor accuracy overall for the conditions tested. The correlation of CO is not shown, as it suffers from similar drawbacks.

![Figure 5.2](image)

**Figure 5.2:** The ALBDF as a function of absorption cross-section for a) H₂O, and b) CO₂. The line-by-line (LBL) calculation is shown with the corresponding orthogonal polynomial correlation (OP). For the data shown, $p = 1$ atm, $Y_i \to 0$, $T_b = 1000$ K, and $T_g$ varies from 400 K to 3000 K, as shown.

Although the orthogonal polynomial correlation form explored here suffers from poor accuracy, it shows promise as an efficient and useful method of representing the ALBDF, primarily due to its simplicity and speed. There are a few directions of future research that could prove fruitful in this regard. First, orthogonal polynomials could be used in piecewise form in combination with a method of representing the ALBDF that has better accuracy at high
absorption cross-section, where small losses of accuracy in the ALBDF have the potential of causing significant inaccuracy in calculations of radiative transfer. Second, orthogonal polynomials could be applied only to a narrow range of parameters (temperature, pressure, and mole fraction). This could be useful for specific research applications where parameters do not vary over the full range investigated in this study. In general, orthogonal polynomials show promise as a correlation form when smaller parameter ranges are required.

### 5.4 Comparison of ALBDF Representations

The updated hyperbolic tangent correlation and tabulated data will now be used in computations of radiation-relevant parameters and compared with line-by-line ALBDF data for each of the three species considered in this study. Example subroutines written in C++ to calculate the ALBDF using the updated correlation or the tabulated data can be seen in Appendix C. Figure 5.3 shows the ALBDF for water vapor as a function of absorption cross-section and total pressure. Shown are the LBL calculation, the ALBDF generated from tabulated data, and the correlation for a) $T_g = T_b = 1000$ K, and b) $T_g = T_b = 3000$ K. The mole fraction of H$_2$O in this case is $Y_{H_2O} = 0.2$. It can be seen that the tabulated data match the LBL solution precisely, whereas the correlation shows some deviation, although the agreement between the correlation and the LBL data is overall very good at these conditions. The impact of differences between correlation and line-by-line generated ALBDF on predicted radiative transfer in several idealized problems will be characterized in Chapter 6. The agreement between the LBL data and the correlation is especially good at high values of absorption cross-section where there is a stronger impact on calculations of radiative transfer.
Figure 5.3: The ALBDF for H$_2$O at a) $T_g = T_b = 1000$ K, and b) $T_g = T_b = 3000$ K. Shown are the line-by-line (LBL) solution, the solution taken from tabulated data, and the correlation. Total pressure is shown, and the mole fraction is $Y_{H_2O} = 0.2$.

The ALBDF for CO$_2$ as a function of absorption cross-section and total pressure is shown in Fig. 5.4 at a) $T_g = T_b = 1000$ K, and b) $T_g = T_b = 3000$ K. Once again, the LBL solution, the ALBDF generated from the tabulated data, and that calculated from the correlation are shown. Because the mole fraction dependence can be neglected, the mole fraction for the LBL data was set to $Y_{CO_2} \rightarrow 0$. Once again, it can be seen that the ALBDF generated from the tabulated data matches the LBL solution extremely well. The correlation also has very good accuracy, although it is seen that there exists a region of poorer accuracy for combinations of high pressure and low gas temperature. A close inspection of the correlation for CO$_2$ reveals that for pressures above 4 atm, some loss of accuracy is expected for low gas temperatures. This region is very small at 8 atm, with only the ALBDF at gas temperatures of 600 K or below being affected. The region of absorption cross-section suffering from poor accuracy grows somewhat as pressure increases, and at 50 atm, the ALBDF at temperatures up to about 1500 K show some loss of accuracy. The
loss of accuracy is primarily seen for low values of absorption cross-section, $C$. Again, the impact of these inaccuracies in the correlated ALBDF on radiative transfer predictions at conditions of practical engineering relevance will be presented in Chapter 6.

![Graph (a)](image1.png)

![Graph (b)](image2.png)

Figure 5.4: The ALBDF for CO$_2$ at a) $T_g = T_b = 1000$ K, and b) $T_g = T_b = 3000$ K. Shown are the line-by-line (LBL) solution, the solution taken from tabulated data, and the correlation. Total pressure is shown, and the mole fraction is approaching zero.

The ALBDF for CO is shown in Fig. 5.5 as a function of absorption cross-section and total pressure for a) $T_g = T_b = 1000$ K, and b) $T_g = T_b = 3000$ K. The line-by-line solution, the tabulated data, and the correlation are shown. As in the case of CO$_2$, the mole fraction dependence of CO is also neglected, so for the LBL solution, $Y_{CO} \to 0$. The tabulated data again match the LBL solution nearly exactly, while the correlation demonstrates accuracy that is overall quite adequate for engineering applications.
**Figure 5.5:** The ALBDF for CO at a) $T_g = T_b = 1000$ K, and b) $T_g = T_b = 3000$ K. Shown are the line-by-line (LBL) solution, the solution taken from tabulated data, and the correlation. Total pressure is shown, and the mole fraction is approaching zero.

The accuracy of the updated hyperbolic tangent correlation is not as good for CO as for H$_2$O and CO$_2$, likely due to the fact that the ALBDF for CO remains near unity for most of the conditions considered in this study, and this presents curve-fitting challenges. Further, the correlation of the ALBDF of CO is not recommended if $T_b - T_g > 2200$ K, as this range of parameters may lead to gray gas weights at high absorption cross-section that can become negative. Gray gas weights, $a_j$, are calculated as the difference between the ALBDF at consecutive values of absorption cross-section, as seen below.

$$a_j = F(C_j, p, T_g, T_b, Y) - F(C_{j-1}, p, T_g, T_b, Y).\quad (5-14)$$

There are other cases where negative gray gas weights are found at very low absorption cross-section, but this has a smaller impact on calculations and can be handled in practice by setting these negative weights to zero.
For all three gas species explored it can be seen that the variation of the ALBDF with absorption cross-section becomes less smooth at higher total pressure. As explained previously, the spectral lines become wider and have lower peaks at increasing total pressure, and therefore, as $C$ increases there are more abrupt changes in the ALBDF than if the spectral lines are tall and narrow at low pressure. This added irregularity results in a modest loss in the accuracy of the correlation for all three species at very high pressure due to the added difficulty in fitting the line-by-line data.

Perhaps the main reason for the loss in accuracy that is seen for the correlation for both CO$_2$ and CO at elevated pressure is the limitations of the hyperbolic tangent correlation form. It is not likely that the same correlation form, applied to three gas species for an extreme range of temperatures and total pressures, would capture accurately the ALBDF behavior at all conditions. This correlation form, extensively developed and widely adopted, gives excellent results for most conditions where radiative exchange is significant and for which the correlation would normally be used in engineering situations. Further, the correlation it is quite simple to implement. When higher accuracy is required, the look-up table approach may be more appropriate.

5.5 Gray Gas Weights

In the SLW method for solution of the radiative transfer equation, the ALBDF is used to calculate gray gas weights, $a_j$. Therefore, it is of interest to observe the behavior of the weights for different conditions. Gray gas weights are calculated as a difference between values of the ALBDF found at adjacent absorption cross-sections, as seen in Eq. (5-14).

The variation of the gray gas weights with absorption cross-section depends on the number of gray gases employed. Values of $a_j$ found rigorously using the line-by-line (LBL)
calculation of the ALBDF are compared with those found using the tabulated data and the correlation in Fig. 5.6 for a) 10 gray gases, b) 25 gray gases, and c) 71 gray gases (the absorption cross-section resolution used in the generation of the tabulated data). Shown are the weights for \( Y_{H_2O} \to 0, \ T_g = T_h = 1500 \text{ K}, \) and \( p = 50 \text{ atm}. \) These parameters were chosen to illustrate the effect of varying the number of gray gases. For each of the cases shown, the line-by-line solution matches the tabulated data very closely. The correlation generally follows the same trend as the line-by-line data, but the peaks and valleys that are present in the line-by-line data do not appear when using the correlation. The peaks are caused by inflections (positive and negative changes in slope of the \( F - C \) behavior) in the ALBDF. Because the correlation is a smooth approximation of the line-by-line data, the weights are also smoothly distributed with absorption cross-section.

As seen in Fig. 5.6a, when fewer gray gases are used, the distribution of the gray gas weights becomes smoother, with the peaks becoming less apparent or vanishing completely. Also, when fewer gray gases are used the magnitude of the weights increases. This is because the gray gas weights sum to unity, and with more gray gases each weight must necessarily be smaller. Not shown on the plots is the weight of the clear gas, which is required to bring the total of the sum of all gray gases to unity. Typical combustion predictions use approximately 10 gray gases or fewer in order to make calculations computationally feasible, so the distribution in Fig. 5.6a is more likely to be encountered in practice. When the number of gray gases is increased to 25 (Fig. 5.6b), the detailed shape of the variation of gray gas weights with absorption cross-
Figure 5.6: Gray gas weights, $a_j$, calculated using line-by-line data (LBL), the tabulated data, and the correlation for a) 10 gray gases, b) 25 gray gases, and c) 71 gray gases. The data were generated at $Y_{H_2O} \rightarrow 0$, $T_g = T_b = 1500$ K, and $p = 50$ atm.
section emerges. Increasing the number of gray gases to 71 (Fig. 5.7), the resolution of the tabulated line-by-line data, reveals somewhat more detail, but it can be seen that the difference in behavior between 25 and 71 gray gases is minor. Therefore, the data that follow (Figs. 5.7 to 5.9) will be calculated using 25 gray gases.

The gray gas weights for H₂O are considered in Fig. 5.7. The weights were calculated at $Y_{\text{H}_2\text{O}} \rightarrow 0$ and a) $T_g = T_b = 1500$ K and $p = 1$ atm, b) $T_g = T_b = 1500$ K and $p = 50$ atm, c) $T_g = T_b = 3000$ K and $p = 1$ atm, and d) $T_g = T_b = 3000$ K and $p = 50$ atm. Weights are calculated using the line-by-line data (LBL), the tabulated data, the correlation, and the previous correlation of Denison and Webb (1993b). At elevated pressures, the pressure correction developed by Denison and Webb (1996a) is combined with the atmospheric correlation of Denison and Webb (1993b). As can be seen, increases in temperature lead to the appearance of more peaks in the line-by-line data. Likewise, increasing pressure causes more peaks to appear. For both increases in temperature and pressure, the ALBDF becomes less smooth. This is caused by an increase in line density corresponding to increasing temperature and more abrupt changes in $F$ due to shorter, wider lines corresponding to increasing pressure. For all cases, use of the tabulated data yields weights that are nearly identical to those calculated using the line-by-line data. The new correlation gives an excellent approximation, and captures the shape of the weights generated from the line-by-line calculation very well. The previous correlation of Denison and Webb under-predicts weights at 1500 K. At 3000 K the previous correlation is not valid since it is limited to an upper temperature of 2500 K, and can be seen to perform very poorly when extrapolated in temperature.
Figure 5.7: Gray gas weights of H$_2$O as a function of absorption cross-section calculated at $Y_{H_2O} \rightarrow 0$ and a) $T_g = T_b = 1500$ K and $p = 1$ atm, b) $T_g = T_b = 1500$ K and $p = 50$ atm, c) $T_g = T_b = 3000$ K and $p = 1$ atm, and d) $T_g = T_b = 3000$ K and $p = 50$ atm.

Figure 5.8 shows the gray gas weights for CO$_2$ calculated at $Y_{CO_2} \rightarrow 0$ and a) $T_g = T_b = 1500$ K and $p = 1$ atm, b) $T_g = T_b = 1500$ K and $p = 50$ atm, c) $T_g = T_b = 3000$ K and $p = 1$ atm, and d) $T_g = T_b = 3000$ K and $p = 50$ atm. Weights are again calculated using the line-by-line data (LBL), the tabulated data, the correlation, and the previous correlation of Denison and Webb (1995a), which has once again been combined with the pressure correction (Denison and Webb,
Figure 5.8: Gray gas weights of CO$_2$ as a function of absorption cross-section calculated at $Y_{CO_2} \to 0$ and a) $T_g = T_h = 1500$ K and $p = 1$ atm, b) $T_g = T_h = 1500$ K and $p = 50$ atm, c) $T_g = T_h = 3000$ K and $p = 1$ atm, and d) $T_g = T_h = 3000$ K and $p = 50$ atm.

1996a). For CO$_2$, there doesn't appear to be an increase in the number of peaks with temperature or pressure; rather, the strength of the peaks increases with temperature and pressure. Again it is seen that use of the tabulated data yields weights nearly identical to those calculated using the line-by-line data. The new correlation performs very well for the conditions shown. The previous
correlation of Denison and Webb gives good results at moderate temperature and atmospheric pressure, but the adaptation for variable pressure can lead to poor results, as seen in Fig. 5.8b. This is not surprising since the correction for variable pressure developed previously (Denison and Webb, 1996a) was preliminary and never fully validated. It can be seen once again that use of the previous correlation at 3000 K is inappropriate.

Figure 5.9 presents the gray gas weights for CO calculated at \( Y_{CO} \rightarrow 0 \) and a) \( T_g = T_b = 1500 \) K and \( p = 1 \) atm, b) \( T_g = T_b = 1500 \) K and \( p = 50 \) atm, c) \( T_g = T_b = 3000 \) K and \( p = 1 \) atm, and d) \( T_g = T_b = 3000 \) K and \( p = 50 \) atm. Weights are again calculated using line-by-line data (LBL), tabulated data, and the correlation. No correlation for carbon monoxide has been previously published, so no comparison to previous work is presented. For CO, the weights decrease in strength as temperature increases. This indicates that the weight of the clear gas will be greater at increasing temperature. Once again, use of the tabulated data yields weights nearly identical to those calculated using the line-by-line data. The new correlation performs adequately for the conditions shown, though accuracy is not as good as for the correlation of H\(_2\)O and CO\(_2\), particularly at high pressure. Further, as indicated previously, negative weights at low absorption cross-section can appear for combinations of high temperature and pressure (Fig. 5.9d). In practice, these negative weights can be arbitrarily assigned a zero value to improve accuracy of calculations, as mentioned previously.

When the gray gas weights for the different species are compared, it can be seen that the highest magnitudes are found for H\(_2\)O. Further, the gray gas weights for H\(_2\)O as a function of absorption cross-section rise from values near zero at low absorption cross-section to a peak value, then fall to a value of zero. By contrast, the weights for CO\(_2\) and CO typically begin at an
Figure 5.9: Gray gas weights of CO as a function of absorption cross-section calculated at \( Y_{CO} \rightarrow 0 \) and a) \( T_g = T_b = 1500 \text{ K and } p = 1 \text{ atm} \), b) \( T_g = T_b = 1500 \text{ K and } p = 50 \text{ atm} \), c) \( T_g = T_b = 3000 \text{ K and } p = 1 \text{ atm} \), and d) \( T_g = T_b = 3000 \text{ K and } p = 50 \text{ atm} \).

elevated value (for the minimum absorption cross-section of practical interest) and descend to zero as absorption cross-section increases. These effects are due to the fact that the ALBDF for H\(_2\)O is near zero at the lower limit of absorption cross-section (\( 10^{-4} \text{ m}^2/\text{mol} \)). As a result, the full distribution of gray gas weights is seen, and the magnitudes are higher since the clear gas has a
very small weight. The clear gas for CO frequently has a very high weight, a result of the small magnitudes seen in Fig. 5.9.

5.6 Computation Time Comparison

A significant consideration when choosing between the correlation and the tabulated data is required computation time. It has been mentioned that the interpolation step required in using the tabulated data is significantly faster than using the correlation but that an initial cost to read the data is incurred. Figure 5.10 seeks to characterize the computational cost of the different representations of the ALBDF in practical radiative transfer computations. Shown in Fig. 5.10 is the computation time required for obtaining $N$ values of the ALBDF using an Intel(R) Core(TM)2 Duo CPU E6750 @ 2.66GHz with 2.0 GB RAM. Data are shown for ALBDF calculations using the hyperbolic tangent correlation both at atmospheric pressure [“Correlation (atm. pressure)”] (corresponding to the use of the hyperbolic tangent correlation without including the self-broadening or pressure shifts) and at variable pressure [“Correlation (var. pressure)”]. Data are also shown for ALBDF calculations employing the tabulated data for CO$_2$ or CO (independent of mole fraction) or for H$_2$O (mole fraction dependence included) [“Tables”]. Finally, computation times are given for the orthogonal polynomial correlation of orders 3 and 10 [“OP (order 3)” and “OP (order 10)”]. The orthogonal polynomial correlation used for these measurements included a mole fraction dependence, so it can be expected that the computation times would be equivalent for variable pressure calculations but that it would be lower if there were no mole fraction or pressure dependence.
Figure 5.10: The computation time of a representation of the ALBDF as a function of number of calculations, $N$. Shown are times for the hyperbolic tangent correlation for both the atmospheric correlation and for variable pressure, the time to access the tabulated data for the species investigated, and the orthogonal polynomials of order 3 and 10.

As seen in Fig. 5.10, the computation time for the hyperbolic tangent correlation is significantly less than for the tabulated data when the number of computations is small. At about 500,000 calculations of the ALBDF, the look-up table approach overtakes the hyperbolic tangent correlation and becomes the faster method. The orthogonal polynomial approach is the fastest method for all cases (although suffering significantly lower accuracy in the form investigated here). The third order orthogonal polynomial correlation is about two orders of magnitude faster than the corresponding hyperbolic tangent correlation. It should be emphasized that these results are undoubtedly computer-dependent and/or programming environment-dependent. Significantly faster read-write speeds could reduce the cross-over point at which use of tabulated data would be more efficient than use of the correlation.
5.7 Summary

The ALBDF has been represented through an updated and expanded hyperbolic tangent correlation of the form originally proposed, and through tabulated data. The improvements over previous representations include more rigorous generation of line-by-line data, a wider temperature range, variable total pressure, and the development of ALBDF representations for carbon monoxide. Representing the ALBDF using orthogonal polynomials was also explored, with the conclusion that this correlation method shows promise for applications with more limited conditions. Some representative ALBDF data were given, demonstrating a few potential accuracy issues when using the hyperbolic tangent correlation, although the overall accuracy of the correlation is excellent. The tabulated line-by-line data represent the ALBDF with nearly perfect accuracy with the only inaccuracy being caused by interpolation. Computation of gray gas weights, an important intermediate quantity in the use of the SLW method, further demonstrates the accuracy of the tabulated data and the correlation. The computation times of the three representations of the ALBDF were compared, showing that orthogonal polynomials have the potential to calculate the ALBDF the fastest, with the tabulated data being faster than the hyperbolic tangent correlation after about 500,000 calculations of the ALBDF (for the computer platform used in the study).
6 VALIDATION OF ALBDF REPRESENTATIONS

The SLW method is based on the discretization of the absorption spectrum into a discrete number of gray gases. Each of the gray gases has traditionally been characterized by a gray gas absorption coefficient calculated from the discrete absorption cross-sections as

\[ \kappa_j = NY \sqrt{C_{j-1} C_j} = \left( \frac{p}{R_u T_{g, j}} \right) \left( \frac{P_i}{P} \right) \sqrt{C_{j-1} C_j}, \]  

(6-1)

where the values of absorption cross-section \( C_j \) are, in traditional implementations of the SLW method, logarithmically evenly spaced between \( C_{\text{min}} \) and \( C_{\text{max}} \) and can be calculated using the following equation:

\[ C_j = C_{\text{min}} \left( \frac{C_{\text{max}}}{C_{\text{min}}} \right) \frac{j}{N}. \]  

(6-2)

The index \( j \) in Eqs. (6-1) and (6-2) varies from 0 to \( N \), where \( N \) is the number of gray gases. The values of \( C_{\text{min}} \) and \( C_{\text{max}} \) are the lower and upper limits on absorption cross-section appropriate for the species involved in the problem of interest. As discussed in Chapter 5, somewhat different bounds on absorption cross-section apply to the different species and to the different representations of the ALBDF. If the look-up table is used for any single gas or for mixtures of gases, \( C_{\text{min}} = 10^{-4} \text{ m}^2/\text{mol} \) and \( C_{\text{max}} = 1000 \text{ m}^2/\text{mol} \). For the case where the correlation for the ALBDF is applied to a single participating gas, \( C_{\text{min}} = 10^{-4} \) and \( C_{\text{max}} = 60 \text{ m}^2/\text{mol} \) for H\textsubscript{2}O and CO or \( C_{\text{max}} = 600 \text{ m}^2/\text{mol} \) for CO\textsubscript{2}. When the correlation is used for mixtures of gases, \( C_{\text{max}} \) can be set to 600 m\textsuperscript{2}/mol if CO is excluded since the correlation for H\textsubscript{2}O can be safely extrapolated.
to this value. If CO is an element of the mixture, 60 m$^2$/mol should be used for $C_{max}$, in which case a small loss of accuracy in the representation of CO$_2$ would be possible. For either mixture case, $C_{min} = 10^{-4}$ m$^2$/mol.

The ALBDF is the primary tool for capturing the gas radiative properties in the SLW method. The SLW method is typically used when solving the radiative transfer equation (RTE), but can also be used to calculate total emissivity or other radiative quantities derived from spectral data. The hyperbolic tangent correlation of the ALBDF and the tabulated line-by-line ALBDF data will now be used in calculations of total emissivity and radiative transfer to validate their accuracy. These calculations will be compared to benchmark data in the form of either line-by-line calculations using HITEMP 2010 or experimental data where such data exist.

### 6.1 Total Emissivity

Figure 6.1 shows the total emissivity as a function of temperature for a) H$_2$O, b) CO$_2$, and c) CO using the LBL calculation, the calculation obtained using the updated ALBDF correlation, and the calculation obtained using the tabulated ALBDF data. The ALBDF is used to calculate the gray gas weights when performing total emissivity calculations using the weighted-sum-of-gray-gases model:

$$
\epsilon = \sum_{j=1}^{N} a_j(1 - e^{-\kappa_j L}),
$$

where $N$ is the number of gray gases. The line-by-line calculation for the total emissivity is obtained as described in Section 4.3.

Total emissivity data are calculated at the same conditions as the emissivity data in Fig. 4.10. For the data shown, the pathlength is $L = 1$ m and the mole fraction is $Y_i = 0.01$ unless
otherwise indicated. The additional case with a higher concentration of H\textsubscript{2}O is also included in the figure to illustrate the accuracy of the ALBDF representations for this case.

As can be seen in Fig. 6.1, the look-up table approach again matches the LBL solution precisely for all three species over the full range of temperature and pressure. It can be seen that the correlation is more accurate for H\textsubscript{2}O and CO\textsubscript{2} than for CO. For H\textsubscript{2}O and CO, the poorest accuracy is seen at sub-atmospheric total pressure and elevated temperature, where the total emissivities are very small. For CO\textsubscript{2}, the combination of high pressure and low temperature is seen to yield the least accurate results in the calculations based on the correlation, which agrees with results from Section 5.4.

![Figure 6.1: Total emissivity, $\varepsilon$, as a function of temperature and total pressure for a) H\textsubscript{2}O, b) CO\textsubscript{2}, and c) CO. Shown are line-by-line data, the solution obtained using tabulated data, and the solution obtained using the correlation. For the data shown, $Y_i = 0.01$ unless otherwise indicated.](image)

Comparisons were also made using experimental and experimentally-based total emissivity data available in the literature. A comparison of Fig. 6.1 and Fig. 4.10 show that the
present data for H$_2$O and CO$_2$ show good agreement with the Leckner correlation, which as mentioned in Section 4.3, is experimentally based.

Further total emissivity data for H$_2$O, including a temperature-dependent correction factor for variable pressure, were given by Ludwig et al. (1973). Although these data are somewhat dated, they are semi-empirical. Comparisons with these data were made using the line-by-line formulation (Eq. (4-3)) and the SLW formulation (Eq. (6-3)) using tabulated data and the correlation in Fig. 6.2 as a function of temperature. Shown in Fig. 6.2 are data at $p = 0.1$, 1, and 2 atm and for $pL = 1$ and 100 cm-atm. As can be seen, the data at each partial pressure-

![Figure 6.2: Total emissivity of H$_2$O at $p = 0.1$, 1, and 2 atm and $pL = 1$ and 100 cm-atm as a function of temperature. Shown are data taken from Ludwig et al. (1973), calculated emissivity using line-by-line data, and emissivity generated from tabulated ALBDF data, and the ALBDF correlation.](image_url)
pathlength are grouped, and data at each value of total pressure are represented by a different color (blue for 0.1 atm, black for 1 atm, and red for 2 atm). The calculation using the tabulated data and the correlation match the line-by-line solution very well, although they generally lie above the Ludwig correlation results at sub-atmospheric pressure and below the Ludwig data at pressures greater than atmospheric pressure. The emissivity data for conditions other than \( p = 1 \) atm are in the form of a correction from the correlation result at atmospheric pressure. Therefore, because the agreement is not perfect at atmospheric pressure, it is expected that the data at 0.1 atm and 2 atm will show some disagreement. However, the present calculations follow the same trends as the Ludwig data, and the overall agreement is good.

6.2 Radiative Transfer in Isothermal, Homogeneous Media

To investigate the impact of different representations of the ALBDF in radiative transfer calculations the ALBDF correlation and the tabulated ALBDF data were used in the solution of the RTE for one-dimensional media using the SLW method for a moderate and high temperature case for each gas in a mixture with air. The line-by-line solution serves as benchmark in the comparison. The first test case is for an isothermal medium at \( T = 1250 \) K, \( Y_i = 1.0, p = 0.1, 1, \) or 50 atm, with a layer length of \( L = 1 \) m. The walls have an imposed emissivity of 0.8 and are relatively cold at 400 K. The second test case considers a medium at \( T = 2750 \) K, \( Y_i = 0.4, p = 0.1, 1, \) or 50 atm, and a layer length of \( L = 0.5 \) m. The walls for this case are gray with an emissivity of 0.5 and a temperature of 1000 K. The discrete ordinates method is used to solve the Radiative Transfer Equation in both SLW and line-by-line calculations. This solution method with the pertinent equations and boundary conditions has been described in detail previously (Solovjov and Webb, 2000). In both cases a spatial grid of 200 points was used to discretize the space variable, and 36 ordinates were used in angular discretization. Iterations were continued
until the intensities changed by less than $10^{-16}$ W/m$^2$sr. 20 gray gases were used in the SLW predictions. When 200 spatial intervals are used, the peak divergence has been found to be about 0.16% different from that obtained when 2000 spatial intervals are used.

For the line-by-line calculation of divergence of radiative flux, the Radiative Transfer Equation was solved for intensity within each wavenumber interval, multiplied by the width of the wavenumber interval, and the resulting intensity from all intervals were summed to obtain total radiative intensity. The wavenumber interval was the same as that used to generate the line-by-line ALBDF, $\Delta \eta = 0.005$ cm$^{-1}$. In making this calculation, the absorption coefficient, $\kappa$, is calculated using Eq. (6-1). The same spectral database, including all appropriate cutoff criteria for determining contributions from lines, was used for both line-by-line predictions and SLW simulations.

The divergence of radiative flux, $-dq/dx$, is calculated numerically as the negative derivative of the radiative flux using a central difference approach. The net radiative flux, $q(x)$, is calculated within each spectral interval according to Solovjov and Webb (2000)

$$q(x) = 2\pi \sum_{i=1}^{n} \mu_i w_i [I_i^+(x) + I_i^-(x)], \quad (6-4)$$

where $n$ is the number of ordinates, $\mu_i$ and $w_i$ are the ordinate direction and weight of direction $i$, and $I_i^+$ and $I_i^-$ are intensities in the positive and negative directions. The intensities are calculated from the discrete ordinates method, as described by Solovjov and Webb (2000).

A similar RTE solution approach was applied for the SLW model. However, for this case, the absorption coefficient and gray gas weights are calculated using the ALBDF. Further, the Radiative Transfer Equation is solved for each gray gas instead of within each spectral interval, and the results are summed over all gray gases to yield predictions of the total
quantities. The subroutines needed to calculate the SLW solution to this problem are found in Appendix D.

Figure 6.3 shows the divergence of the total radiative flux if the gas considered is H$_2$O for the case of a) 1250 K, and b) 2750 K. As compared to the benchmark line-by-line simulations, the accuracy for either ALBDF representation is very good, but more particularly when the tabulated data are applied. As total pressure is increased from 1 atm to 50 atm for the 1250 K case it is interesting to note that the magnitude of the divergence of the radiative flux decreases except near the walls. This is because the medium is becoming optically thick for the conditions shown.

![Figure 6.3: Divergence of radiative flux in a layer of H$_2$O at a) $T = 1250$ K, and b) $T = 2750$ K. Shown are the line-by-line (LBL) solution and the solution obtained using tabulated ALBDF data or using the correlation. Total pressures of 0.1 atm, 1 atm, and 50 atm are shown.](image)

The solution to the RTE when CO$_2$ is the species of interest is shown in Fig. 6.4 for the same conditions explored in Fig. 6.3. Shown is the total radiative flux divergence for the case of a) $T = 1250$ K, and b) $T = 2750$ K. As with the H$_2$O predictions, the solutions obtained using
tabulated data are nearly identical to the line-by-line solutions. The correlation shows some inaccuracy at the extreme pressure of 50 atm primarily for the lower temperature case. This is consistent with the inaccuracy described in Section 5.4.

![Figure 6.4: Divergence of radiative flux in a layer of CO$_2$ at a) $T = 1250$ K, and b) $T = 2750$ K. Shown are the line-by-line (LBL) solution and the solution obtained using tabulated ALBDF data or using the correlation. Total pressures of 0.1 atm, 1 atm, and 50 atm are shown.](image)

The solution to the RTE when CO is the species considered is shown in Fig. 6.5. The flux divergence is illustrated for the case of a) $T = 1250$ K, and b) $T = 2750$ K. As before, the solution obtained using tabulated data is nearly identical to the LBL solution. Inaccuracies are greater between the correlation and the LBL benchmark for CO. The correlation shows greater inaccuracy at high pressure for CO as well, and this inaccuracy is higher at lower temperature.

As seen in Figs. 6.1, 6.4, and 6.5 and as observed previously, although use of the ALBDF correlation for CO$_2$ and CO can lead to some inaccuracy at combinations of low temperature and high pressure, it should be mentioned that the conditions yielding poorer accuracy are less likely to be encountered in practical engineering situations. Low temperatures and high total pressures
can occur, but are less typical of combustion applications. If such conditions are anticipated, it may be prudent to adopt the use of the tabulated data representation of the ALBDF.

Figure 6.5: Divergence of radiative flux in a layer of CO at a) \( T = 1250 \) K, and b) \( T = 2750 \) K. Shown are the line-by-line (LBL) solution and the solution obtained using tabulated ALBDF data or using the correlation. Total pressures of 0.1 atm, 1 atm, and 50 atm are shown.

6.3 Radiative Transfer in Non-isothermal, Non-homogeneous Media

The correlation and the tabulated data are next applied to a gas layer that is non-isothermal and non-homogeneous. For this case, some additional approximations must be made when applying the SLW model. First, the multiplication approach was invoked to treat the mixture of gases (Solovjov and Webb, 2000). Next, the reference approach was used to account for spatial variations in the temperature and mole fraction (Denison, 1994). Because these models have been applied, the difference between the LBL solution and the SLW solutions must be attributed to the combined effect of the approximate approaches used to treat the mixture and inhomogeneity and any error caused by the representation of the ALBDF. The discrete ordinates
model was again used with the same specifications as described above. The SLW method, including the reference approach and multiplication method, was applied using the subroutines in Appendix E.

The first case considered here follows a test case from Solovjov and Webb (2000). For this case, the one-dimensional medium has a length of \( L = 1 \) m, with temperatures and mole fractions following a spatial stepwise variation as shown below:

\[
T = 1000 \text{ K}; \quad Y_{\text{H}_2\text{O}} = 0.2; \quad Y_{\text{CO}_2} = 0.1; \quad Y_{\text{CO}} = 0.03 \quad \text{if } 0 \text{ m} \leq x \leq 0.35 \text{ m},
\]

\[
T = 1500 \text{ K}; \quad Y_{\text{H}_2\text{O}} = 0.4; \quad Y_{\text{CO}_2} = 0.2; \quad Y_{\text{CO}} = 0.06 \quad \text{if } 0.35 \text{ m} < x < 0.65 \text{ m},
\]

\[
T = 1000 \text{ K}; \quad Y_{\text{H}_2\text{O}} = 0.2; \quad Y_{\text{CO}_2} = 0.1; \quad Y_{\text{CO}} = 0.03 \quad \text{if } 0.65 \text{ m} \leq x \leq 1.0 \text{ m}.
\]

The walls that bound the medium are at a temperature of 1000 K and are gray with emissivity 0.8. The stepwise temperature and concentration configuration makes the line-by-line solution more reasonable to obtain since generation of the full absorption spectrum for the three species is required only at the two thermodynamic states describing the three spatial regions. The second stepwise case considered is identical to the first, with the exception of the imposed gas and wall temperatures. The medium temperatures in the spatial step regions are set to 2000 K and 3000 K, to replace 1000 K and 1500 K, respectively. Likewise, the wall temperature is increased to 2000 K. The code used to calculate the line-by-line solution for this problem can be found in Appendix F. This code can be simplified to solve the homogeneous, isothermal problems considered in this work, such as the cases presented in the previous section.

Figure 6.6 shows the predicted divergence of the radiative flux as a function of position for a) the lower temperature case, and b) the high temperature case. The left panel shows the solution for total pressures of 0.1 and 1 atm, while the right panel shows the 50 atm case. As can be seen, at these conditions the accuracy of the SLW model is excellent when either the
correlation or the tabulated data are applied. The average error is 9% when the correlation is applied and 5.8% when the tabulated data are applied. The accuracy of the correlation in the case of higher temperature is not as good as it is for more moderate conditions, particularly for sub-atmospheric pressure where the average error is 65%, but is less than 10% for the other two total pressures. The average error is 8.7% when the tabulated data are applied to the higher temperature case.

Figure 6.6: Divergence of radiative flux at 0.1, 1, and 50 atm in a gas mixture exhibiting a stepwise temperature and concentration profile for a) 1000K and 1500 K, and b) 2000 K and 3000 K. Shown are the line-by-line (LBL) solution, the solution obtained using the tabulated data, and the solution obtained using the correlation.
6.4 The BERL Experiments

The accuracy of the use of tabulated data and correlation representations of the ALBDF in predicting radiative transfer will now be validated using experimental data taken from laboratory-scale combustion experiments where natural gas was burned in air. Lallemant et al. (1996) report intensity measurements in a vertically-fired furnace in the Burner Engineering Research Laboratory (BERL) at Sandia National Laboratories in Livermore, California (Sayre et al., 1994a; Sayre et al., 1994b). The burner is approximately 1.2 m in diameter and is fired from the bottom. Intensity measurements are reported at two axial distances from the burner, and for two wall conditions, resulting in four sets of experimental data. The axial locations at which data were reported are \( \frac{AD}{D_0} = 0.31 \) and 1.25 (where \( AD \) is the axial distance and \( D_0 = 87 \) mm), and the wall temperatures are \( T_w = 300 \) K and 758 K. Local gas temperature and concentration data were reported in the study, and the radial profiles have been imposed here for SLW model predictions. The temperature measurements are shown in Fig. 6.7 for a) the cold wall cases, and b) the hot wall cases. Mole fraction measurements for \( \text{H}_2\text{O}, \text{CO}_2, \) and \( \text{CO} \) are shown in Fig. 6.8 for a) the cold wall cases, and b) the hot wall cases. The flame is reported as non-luminous for these experiments, so the influence of soot and particles is not present in the measurements.

Similar to the cases presented in Section 6.3, the reference approach and multiplication method have been applied to treat the inhomogeneity and mixture of gases. Results can be seen in Fig. 6.9 where the BERL experimental intensity measurements are presented along with their respective SLW predictions, with the ALBDF calculated using tabulated data. Calculations employing the correlation are nearly identical to the prediction obtained using tabulated data, so they are not given. Shown are a) \( T_w = 300 \) K (cold walls) and \( T_w = 758 \) K (hot walls) at \( \frac{AD}{D_0} = 0.31 \), and b) cold and hot wall conditions at \( \frac{AD}{D_0} = 1.25 \). Because the reference approach is
Figure 6.7: The experimental temperature measurements taken from the BERL reactor for a) the cold wall cases, and b) the hot wall cases. The solid lines represent data measured at $AD/D_0 = 0.31$ and the dashed lines represent measurements taken at $AD/D_0 = 1.25$.

Figure 6.8: The experimental mole fraction measurements for H$_2$O, CO$_2$, and CO taken in the BERL reactor for a) the cold wall cases, and b) the hot wall cases. The solid lines represent data measured at $AD/D_0 = 0.31$ and the dashed lines represent measurements taken at $AD/D_0 = 1.25$. 
sensitive to the choice of reference temperature, SLW intensity data are given at two reference temperatures. A standard choice (used in all previous predictions where the reference approach was applied) is to use the volumetric average, \( T_{avg} \) (Denison, 1994). For comparison, the maximum local temperature, \( T_{max} \), was also used as the reference temperature in calculations.

As can be seen in Fig. 6.9, the SLW predictions match the experimental data particularly well for the hot wall conditions at \( AD/D_0 = 1.25 \) (Fig. 6.9b). For the other cases, the SLW predictions, while not demonstrating as good agreement, follow the same trends as the experimental data. For the hot wall cases at both axial locations, changing the reference temperature has a negligible effect on calculations. However, the cold wall cases show sensitivity to the choice of reference temperature, with the prediction improving somewhat at \( AD/D_0 = 0.31 \). It can be assumed that if the reference temperature is reduced that the comparison between SLW predictions and experimental data will improve at \( AD/D_0 = 1.25 \).

Interestingly, a comparison of the experimental data for the cold wall cases shows an increase in radiative intensity by almost a factor of two going from \( AD/D_0 = 0.31 \) to \( AD/D_0 = 1.25 \), even though temperature and concentration profiles are very similar. This gives rise to questions about the experimental error for these cases. Unfortunately, the experimental uncertainty was not characterized in the study (Lallemant, 1996). Regardless, it can be concluded that overall the SLW model can be used with confidence using either the tabulated data or the correlation when making predictions of radiative transfer in comprehensive combustion systems. Further, the reference approach must be used with care since predictions show sensitivity to the choice of reference temperature, particularly when the walls are at a lower temperature.
Figure 6.9: Comparison of experimental radiative intensity measurements and SLW predictions as a function of distance from the furnace wall for a) $AD/D_0 = 0.31$ and b) $AD/D_0 = 1.25$. Shown are data for the case of both cold walls ($T_w = 300$ K) and hot walls ($T_w = 758$ K), as indicated.
6.5 Comprehensive FLUENT Predictions

A second case where experimental data have been reported in the literature was used to validate the correlation and tabulated data. In addition to one-dimensional SLW predictions, a comprehensive CFD simulation was formulated to demonstrate the use of the SLW model in a comprehensive combustion prediction environment, and to assess its accuracy. The data used for comparison are taken from Andersson et al. (2008) where oxy-combustion experiments were reported using propane as the fuel. Flue gas is cooled, dried, and re-injected into the furnace as the diluent for the oxygen in place of the nitrogen that is present in air-fired flames. Because nitrogen is radiatively non-participating, oxy-combustion is a case where accurately treating the contribution of radiative heat transfer is particularly important due to very high concentration of CO₂, a radiatively participating gas. The test facility is cylindrical, with a diameter of 0.8 m and a length of 2.4 m, and is fired downward. Three sets of experimental data were reported by Andersson et al., but two of the experimental conditions yielded very luminous flames and therefore, radiative transfer in these cases are strongly influenced by the presence of soot. The remaining case is only slightly luminous, and thus is influenced by soot to a much lesser extent. It is this latter case that is used as validation here. The contribution to radiative transfer from soot is assumed to be weak and is neglected in all calculations of the turbulent combustion.

The propane burner is configured as shown in Fig. 6.10 with a fuel lance (diameter = 34 mm) and two cylindrical feed-gas registers. The primary register is swirled with a fin angle of 45 degrees and has an outer diameter of 52 mm. The secondary register is swirled with a fin angle of 15 degrees and has an outer diameter of 92 mm. For the case used in this simulation, the recycled flue gas is 21% oxygen (by volume) when it is injected into the burner at 300 K. The flow rate for the primary oxidant register is 37 m³/h at standard conditions and for the second
register is 54 m$^3$/h at standard conditions. Enough fuel was injected to reach a stoichiometric ratio of 1.15.

![Figure 6.10: The propane burner used by Andersson et al. (2008).](image)

The walls of the furnace were refractory-lined, and four cooling tubes of unknown dimensions and temperatures were inserted axially along the walls and equally spaced circumferentially in the furnace, to cool the flame. Wall temperature was not reported in the study. Consequently, the effective wall temperature from these two effects was assumed to be about 823 K, since using this as a boundary condition in FLUENT yields gas temperatures near the measured values, as will be shown.

A FLUENT simulation was formulated using the conditions described above. The swirl was included by imposing axial and tangential components of the inlets near the fin angles given in the paper. The exact angles were not used since typically the fins in swirl registers are not large enough to fully redirect the flow. Because of this, the primary oxidant was injected 60% in the axial direction and 40% in the tangential direction and the secondary oxidant was injected 80% in the axial direction and 20% in the tangential direction. Walls were set to 823 K, as
mentioned, with an assumed emissivity of 0.8. The mass-flow inlets for both fuel and oxidizer were set to 300 K and appropriate mass-flow rates as described above. The flow field was assumed to be turbulent using the $k-\varepsilon$ model, and the chemical reaction was modeled using a two-step propane combustion model. The turbulence-chemistry interactions were modeled using the eddy-dissipation model. The discrete ordinates radiation model was used, with 4 divisions in theta and phi, 2 pixels in theta and phi, and 10 gray gases. The SIMPLE scheme was used in calculations, along with first-order upwind approximations.

A User-Defined Function (UDF) was written to implement the SLW model incorporating both the correlation and the tabulated data. The multiplication method and the reference approach were again applied to treat the mixture of gases and the inhomogeneity. In addition to simulations incorporating the SLW method, the classical weighted-sum-of-gray-gases (WSGG) model (Smith *et al*., 1982) was also implemented. This was done to compare the recommended gas radiation property model in FLUENT with the SLW method. When implementing the WSGG model, the same specifications are used as in the SLW predictions except now, the absorption coefficient and gray gas weights are calculated according to the WSGG model. Shown in Fig. 6.11 is the axisymmetric mesh used in the simulation. The colored lines indicated in Fig. 6.11 show the inlet (red), the outlet (blue), and the two locations where experimental measurements were provided in the paper (green): at 384 mm and 1400 mm from the burner.

Iterations were carried out until residuals either ceased to change or fell below $10^{-5}$. Although the process of implementing the SLW method in FLUENT using the tabulated data is very similar to using the correlation, it was found that iterations are about 25 times faster when the tabulated data are used compared to the simulations using the correlation. This significant difference was surprising, and is likely because use of the tabulated data requires only algebraic
operations. For the WSGG model, iterations were approximately five times faster than the case where the tabulated data are used.

Figure 6.11: The mesh used in FLUENT simulations. Shown on the mesh are the burner region (red), the furnace exit (blue), and at 384 mm and 1400 mm, the locations where experimental data were reported (green lines).

Figure 6.12 shows the steady-state temperature field for the FLUENT simulation incorporating the WSGG radiation property model. Temperatures range from room temperature (27°C) up to 1400°C in the flame. Figure 6.13 shows the temperature fields generated when the SLW method was used incorporating either a) the tabulated data, or b) the correlation. The temperature fields in both Fig. 6.12 and Fig. 6.13 show cold gas entering the furnace, a flame region, recirculation regions around the flame, and products of combustion that are cooled by the walls as they move downstream. It can be seen from a comparison of Fig. 6.12 and Fig. 6.13 that the much simpler WSGG model yields a relatively similar temperature profile compared to the more complex SLW method. However, the peak temperature is over-predicted by up to 43°C when the WSGG model is implemented compared to the SLW predictions. The SLW predictions seen in Fig. 6.13 are quite similar qualitatively. The simulation employing the correlation
produced a slightly longer flame region and a peak temperature 18 degrees less than when the tabulated data were used.

A comparison was made between the experimental temperature and mole fraction distributions and those predicted by FLUENT simulations. Figure 6.14 shows the temperature distribution at axial locations of a) 384 mm, and b) 1400 mm from the burner. Shown are data from experiments and from each of the three FLUENT simulations. Similarly, Fig. 6.15 shows the profile of the mole fraction of H₂O, and Fig. 6.16 shows the mole fraction of CO₂. As can be seen, the three FLUENT simulations yield very similar distributions for these quantities. The SLW predictions are particularly close together, with the WSGG model giving slightly different results. The sharper temperature gradients in the flame region and the non-uniform conditions

![Figure 6.12: The temperature field in degrees C resulting from the FLUENT simulation when the WSGG model was implemented.](image-url)
Figure 6.13: Temperature distributions of the FLUENT simulation in degrees C in which the SLW method was used incorporating a) the tabulated data, and b) the correlation.
downstream that are seen in the FLUENT predictions (see Fig. 6.14) indicate a much longer flame region than was present when the experimental data were taken. Although the temperature gradients are not as sharp for the experimental data, it must be recognized that experimental temperature measurements often tend to yield local spatially averaged values. If this is the case, the agreement with experiments could be much better than what is seen in Fig. 6.14. Unfortunately, experimental uncertainty for the measurements was not given.

The mole fraction distributions of H$_2$O predicted by FLUENT are similar to the experimental values at both measurement locations, as seen in Fig. 6.15. The study by Andersson et al. (2008) reports that concentration profiles of H$_2$O and CO$_2$ are nearly uniform at the stoichiometric composition at 1400 mm from the burner, and this is represented by the horizontal black lines instead of data points in Figs. 6.15b and 6.16b because specific data points were not given. The FLUENT simulations, on the other hand, have not yet reached uniform conditions at this point, although the gradients appear to be smoother. The FLUENT predictions for mole
fraction of CO\(_2\) at 384 mm from the burner show the most difference when compared with experimental measurements, although this difference is small considering the very high concentrations of CO\(_2\).

Figure 6.15: H\(_2\)O mole fraction distributions at a) 384 mm, and b) 1400 mm downstream from the burner. Data are given for the experimental measurements and for each of the three FLUENT simulations.

Figure 6.16: CO\(_2\) mole fraction distributions at a) 384 mm, and b) 1400 mm downstream from the burner. Data are given for the experimental measurements and for each of the three FLUENT simulations.
The differences seen when comparing the experiments to the FLUENT predictions illustrated by Figs. 6.14, 6.15, and 6.16 may well be the result of the difficulty in modeling turbulence and swirl. Further, there are some aspects of the geometry that are not adequately described in the experimental study by Andersson et al. (2008), such as the dimensions of the cooling rods, the location and size of the outflow from the furnace, and the emissivity of the walls. Also, experimental uncertainty may be a factor in some areas, such as temperature measurements and steadiness of the flame.

Experimental measurements of radiative intensity were also provided. Because FLUENT does not give intensity in a single angular direction as an option, a one-dimensional SLW prediction using the experimental temperature and concentration measurements was performed for this comparison. The SLW method once again incorporated the multiplication method and reference approach, as well as the discrete ordinates method. The experimental study reports that a cooled black surface was used as a target when intensity measurements were taken, so black walls at 300 K were imposed in the SLW calculation. Figure 6.17 displays the radiative intensity data as a function of position at a) 384 mm from the burner, and b) 1400 mm from the burner. Experimental measurements, along with SLW predictions incorporating the tabulated data and the correlations are given. SLW predictions match the experimental data very well at 384 mm. The SLW simulations over-predict the intensity downstream of the flame at 1400 mm by up to 30%, although qualitative agreement is good.
Figure 6.17: The radiative intensity measured at a) 384 mm, and b) 1400 mm from the burner. Shown are experimental measurements and SLW predictions implementing the tabulated data and correlation.

Calculations of the divergence of radiative flux were also made both from the one-dimensional SLW predictions and the FLUENT simulations implementing the SLW method. Shown in Fig. 6.18 are the predictions for the divergence of radiative flux at a) 384 mm, and b) 1400 mm from the burner. The one-dimensional SLW prediction (implemented using both the
Figure 6.18: The divergence of radiative flux, $-dq/dx$, as a function of position a) in the flame region (384 mm), and b) downstream of the flame (1400 mm). Data are given for the FLUENT simulations implementing the SLW method and for one-dimensional SLW predictions, both of which are implemented using both the tabulated data and the correlation.
tabulated data and the correlation) is based on the experimentally-measured temperature and concentration profiles while the FLUENT calculations correspond to the predicted profiles of Figs. 6.14 to 6.16. Similar to the sharp gradients in Fig. 6.14a, the flux divergence predicted by FLUENT using the SLW model in the flame region varies sharply with position. The divergence implementing the experimental temperature and mole fraction measurements do not reach magnitudes as high as those in the FLUENT simulations in the flame region (Fig. 6.18a), but follows similar trends. Surprisingly, the divergence predicted when the WSGG model was applied is quite similar to the one-dimensional predictions except near the wall. However, considering the temperature and concentration profiles are so similar to the other FLUENT predictions, it is clear that the WSGG model drastically underpredicts the divergence of radiative flux in the flame region. Overall, the FLUENT simulation implementing the SLW method and the experimental measurements show good qualitative agreement. Downstream of the flame (Fig. 6.18b), the FLUENT predictions are significantly different from the one-dimensional SLW predictions. This is a result of the long flame region that was discussed earlier.

6.6 Summary

The efficient representations of the ALBDF developed in Chapter 5 have been utilized to calculate total emissivity and to make predictions of radiative transfer in standalone radiation and coupled comprehensive combustion calculations. These predictions have been compared to benchmark data to validate the new representations of the ALBDF.

Calculations of total emissivity show excellent agreement with line-by-line emissivity data, except for a limited range of conditions where use of the correlation leads to error, such as combinations of low gas temperature and high pressure for CO₂ and overall poorer accuracy for CO, particularly when \( T_b - T_g > 2200 \) K. The implementation of the tabulated data yields
predictions that agree with line-by-line solutions almost exactly. Experimentally-based emissivity correlations of Leckner et al. (1972) and Ludwig et al. (1973) were also used to validate the correlation and tabulated ALBDF data. The SLW calculations showed good agreement with these correlation data.

Line-by-line solutions for radiative transfer were also used to validate the correlation and tabulated data, both in homogeneous, isothermal media and non-homogeneous, non-isothermal media. For the homogeneous, isothermal case, the prediction employing the tabulated data matched the line-by-line solution exactly. The simulation employing the correlation also displayed excellent accuracy, although some inaccuracy was evident for extreme conditions not likely to be encountered in most practical engineering applications. For the case of non-homogeneous, non-isothermal media, there was some error expected due to the introduction of approximation in the simulations to treat the non-isothermal, non-homogeneous gas mixtures. The reference approach and the multiplication method proposed previously were used in the simulations reported here. Despite these additional sources of possible error, the calculations employing the correlation and tabulated data both demonstrated excellent agreement with line-by-line benchmark data. The most significant error seen was for the case where the correlation was used in the combination of high temperature and sub-atmospheric pressure.

Experimental radiative intensity measurements in a laboratory-scale combustor were also compared to SLW calculations. The BERL experiments (Lallemand et al., 1996) reported radiative intensity measurements collected in a furnace where natural gas was burned in air. The measurements were taken for two wall conditions and at two axial locations. The comparison of experimental data with SLW predictions showed very close agreement for one of the datasets, and modest error for the other three. Sensitivity to the choice of reference temperature employed
in the reference approach for treating the non-isothermal, non-homogeneous nature of the layer was characterized. Overall, the comparison gives confidence in the accuracy of the correlation and tabulated data.

The final validation step was to run a full CFD simulation matching conditions for laboratory-scale burner experiments undertaken by Andersson et al. (2008). These oxy-combustion experiments included a propane burner using recycled CO₂ as the diluent. The need to model turbulent mixing and reacting flow, and uncertainty in the swirl configuration rendered difficult the simulation. Not surprisingly, exact agreement between prediction and experimental data was not achieved, as demonstrated by a comparison of predicted and experimentally reported temperature and concentration data. However, good qualitative agreement was obtained when the SLW method was applied. Use of a recommended FLUENT radiation model lead to an over-prediction of peak temperature and an under-prediction of divergence of radiative flux. The SLW method was also applied simply to the one-dimensional intensity data reported in the experiments. This calculation showed good agreement with the experimental intensity measurements, particularly in the flame region.

The correlation of the ALBDF and the tabulated line-by-line data have been robustly validated, and it is believed that they can be used with confidence in predictions of radiative transfer or total emissivity.
7 CONCLUSIONS

The Spectral Line Weighted-sum-of-gray-gases (SLW) method has been demonstrated to be an easily-implemented, accurate method for addressing the strong spectral properties of gases in the prediction of radiative transfer. It has previously been successfully developed and implemented for predicting radiative intensity (and consequently radiative flux and divergence) for cases that are homogeneous or non-homogeneous, isothermal or non-isothermal, and for mixtures of gases. Special cases, such as the exact limit or the case of one optimized gray and clear gas, have also been successfully explored. However, the Absorption Line Blackbody Distribution Function (ALBDF), which is an essential element of the SLW method, was first developed based on a spectroscopic database that has been significantly improved. Further, the ALBDF as originally presented required extension to variable total pressure, higher temperature, and more species of relevance in combustion environments (CO). Robust validation of the SLW method with an updated ALBDF was an area where further research was needed. Addressing these shortcomings has been the focus of this dissertation.

The technical approach to generating the line-by-line spectral absorption cross-section has been described in detail. The HITEMP 2010 database is used as the spectroscopic basis for generating the absorption spectrum. The Voigt line profile has been employed. The contribution of a given spectral line is added to all spectral locations where it has a significant contribution. A cutoff value that determines when a spectral line is no longer significant has been applied.
Further, a cutoff value determining which lines are not sufficiently strong to contribute to the resulting absorption cross-section spectrum has been applied. Because the Lorentz line profile, the dominant element of the Voigt profile for the conditions in this study, is known to lose accuracy in the far-wing region, the contribution of line wings is restricted to a specified distance from the line center. This distance was determined using models that are based on empirical data. The method for extending the rigorous line-by-line absorption cross-section development to mixtures of participating gases has been described. This method includes a summation of the contributions to the absorption cross-section of each gas in the mixture weighted by its mole fraction such that the mixture can be treated as a single gas. The effect of line broadening due to the presence of other species has also been investigated. Based on this investigation, it is recommended that the line broadening by other gases present be treated as air-broadening. This novel and rigorous method for generation of the spectral absorption cross-section is one of the contributions of this work.

The ALBDF for the three species of primary interest in combustion systems, H₂O, CO₂, and CO, was generated over a wide range of gas and blackbody temperature, mole fraction (where appropriate), and total pressure. The ALBDF showed a shift to lower values as total pressure is increased. This shift was observed to be weaker at high temperature. Further, the previously documented shift due to increase in mole fraction of the species of interest was similar to that observed at atmospheric pressure and at high pressure. Finally, the ALBDF was shown to become less smooth as total pressure increases. Understanding the behavior of the ALBDF at variable total pressure is an area not adequately explored previously and has thus been addressed in this work.
Total emissivity calculations were presented for variable total pressure, and it was observed that pressure changes alone account for a significant change in emissivity and a modest change when partial pressure-pathlength is held constant.

Total radiative flux and radiative flux divergence were predicted for a one-dimensional, isothermal layer for both constant length and constant mass cases, revealing that total pressure changes result in a significant impact on radiative transfer. It can be concluded that total pressure changes alone can have a significant impact on radiative transfer in high temperature gaseous media. At a layer temperature of 1000 K the flux exiting a radiating gas layer of fixed mass exhibits a greater than four-fold increase with an increase in pressure from 0.1 to 50 atm as a result solely of associated changes in radiative property of the layer medium. The relative increase in exiting radiative flux is significantly lower for a layer temperature of 2500 K, except in the case of CO. Therefore, the change in the ALBDF for variable total pressure can also be considered of significant importance, with diminishing relative influence at increasing temperature for H$_2$O and CO$_2$.

Comparisons were made of the ALBDF generated based the updated spectral database with that published previously (Denison, 1994). Similarly, the previous and updated ALBDF have been used in the prediction of radiative transfer. These comparisons showed a substantial difference between the updated results and the original results of Denison (1994). The ALBDF calculations from Denison for H$_2$O lie above those calculated using HITEMP 2010. The difference is smaller for CO$_2$, although still significant enough to lead to errors up to 20% in calculations of radiative transfer. The conclusion of this comparison is that the previous correlations of the ALBDF (Denison and Webb, 1993b; Denison and Webb, 1995a), while quite accurate, warranted an update using the new HITEMP 2010 database.
The ALBDF has been represented through an updated and expanded hyperbolic tangent correlation of the form originally proposed, and through tabulated data. The improvements over previously published ALBDF data include more rigorous generation of line-by-line information, a wider temperature range, variable total pressure, and the development of ALBDF representations for carbon monoxide. The new correlation coefficients have been given, and the tabulated data can be accessed through http://albdf.byu.edu. Representing the ALBDF using orthogonal polynomials was also explored, with the conclusion that this correlation method may show promise for applications under more limited conditions. Some representative ALBDF data were given, demonstrating a few conditions where the hyperbolic tangent correlation may suffer modest inaccuracy, although the overall accuracy of the correlation is excellent. The tabulated line-by-line data represent the ALBDF with nearly perfect accuracy with the only inaccuracy being introduced by the required interpolation.

Gray gas weights, an important intermediate quantity in the SLW method, were calculated to further demonstrate the accuracy of the tabulated data and the correlation. The computation times of the three different representations of the ALBDF were compared, showing that the ALBDF is computed using tabulated data more quickly than when computed using the hyperbolic tangent correlation after about 500,000 calculations of the ALBDF.

The efficient representations of the ALBDF have been utilized to calculate total emissivity and to predict radiative transfer in select idealized example cases. These calculations have been compared to benchmark data to validate the new representations of the ALBDF. Calculations of total emissivity show excellent agreement with emissivity data from line-by-line calculations, except for limited conditions where use of the correlation leads to modest error, such as combinations of low temperature and high pressure for CO₂. The implementation of the
tabulated data matched the line-by-line solution nearly exactly for all conditions. Experimentally-based emissivity correlations at various temperatures and pressures were also used to validate the correlation and tabulated data. The SLW calculations showed good agreement with the experimental data.

Line-by-line benchmark solutions for radiative transfer were also used to characterize the accuracy of predictions implementing the correlation and tabulated data for the ALBDF, both in homogeneous, isothermal media and non-homogeneous, non-isothermal media. For the homogeneous, isothermal case, the calculation employing the tabulated ALBDF data matched the line-by-line solution exactly. The calculation employing the correlation also displayed excellent accuracy, although again, minor inaccuracy was seen for some extreme conditions not likely to be encountered in engineering applications. For the case of non-homogeneous, non-isothermal media, there was some error expected due to the use of the reference approach and the multiplication method approximations used to treat the non-isothermal/non-homogeneous gas and gas mixtures. Even so, the calculations employing the correlation and tabulated data both demonstrated excellent agreement with line-by-line benchmark simulations. The most significant error seen was for the case where the correlation was used in the combination of high temperature and sub-atmospheric pressure.

Experimental radiative intensity measurements were also compared to SLW calculations. The BERL experiments (Lallemand et al., 1996) reported radiative intensity measurements acquired in a laboratory-scale furnace where natural gas was burned in air. The measurements were taken for two wall temperatures and at two axial locations. The comparison of experimental data with SLW predictions showed very good agreement for two of the datasets, and some error
for the other two. Overall, this comparison gives confidence in the accuracy of the correlation and tabulated data.

The final validation step was to undertake a full CFD simulation matching conditions for experiments done by Andersson et al. (2008). These oxy-combustion experiments included a propane burner using recycled CO₂ as the diluent. Due to the need to model turbulent transport and reaction, and uncertainty in the swirl configuration, exact agreement with experimental data was not achieved, as demonstrated by a comparison of local gas temperature and concentration profiles. However, good qualitative and reasonable quantitative agreement in temperature and concentration profiles was obtained in the flame region, with poor agreement seen in the downstream location due to a longer flame region predicted by FLUENT. The SLW method was also applied simply to the one-dimensional intensity data reported in the experiments. This calculation showed good agreement with the experimental intensity measurements, particularly in the flame region.

The correlation of the ALBDF and the tabulated line-by-line data have been robustly validated, and it is believed that they can be used with confidence in predictions of radiative transfer.
REFERENCES


APPENDIX A.  LINE-BY-LINE ABSORPTION CROSS-SECTION CODE

The C++ code used to calculate the line-by-line spectral absorption cross-section data, following the development in Chapter 3, is given here. The code shown here is for H$_2$O, and the codes for CO$_2$ and CO are essentially simplifications of this code and are therefore not given.

```cpp
//======================================================
// Read H2O database and make absorption cross-section
// calculations for given conditions.
// John Pearson

#include<iostream>
#include<math.h>
#include<cmath>
#include<fstream>
#include<vector>
#include<string>
#include<complex>
#include<sstream>
using namespace std;

double partition(double T);
void voigt(double& s, double& bl, double& bd, double deta, double& keta);
double WWW(complex<double> Z);
void locate(vector<double>& xx, int n, double x, int& j);

int main()
{
    // Variable declarations
    double T, Y[9], P, dx, cutoff, cutoff2, etalow, etahigh;
    double c2, Tref, Q, piece, delta, deta;
    double s, E, Eta, gammaair, gammaself, n, cutgamma;
    int i, ii, j, jj, TLN, NG, currentsize, check;
    int Ti, Pi, Yi;
    string filein;
    ifstream inFile;

    // Specify values
    dx=0.005; // cm-1 spectral spacing for results
```
cutoff=1e-27;  // cutoff value for intensity

cutoff2=1e-29;  // cutoff for inclusion of contribution

cutgamma=2750;  // number of half-widths to include per line

// Wavenumber Range to cover
etalow=0;
etahigh=25000;

// Constants
c2=1.43878;  // cm K (2nd radiation constant = hc/k)
Tref=296;  // K

vector<double> S(1000000), eta(1000000), gamma(1000000), gamma_D(1000000);
currentsize=1000000;

// mole fractions
Y[0]=0;  Y[1]=0.05;  Y[2]=0.1;  Y[3]=0.2;

T=2500;
P=50;

// Get ratio of total internal partition functions
Q=partition(T);

// Loop over mole fraction
for (jj=0; jj<9; jj++) {

    // Set filename to output data
    Ti=T;  Pi=P;  Yi=10*Y[jj];
    std::ostringstream OutFile;
    if (P==0.1) {
        if (jj==1) OutFile << "Cabs h2o " << Ti << " K Y05 P01.txt";
        else OutFile << "Cabs h2o " << Ti << " K Y " << Yi << " P01.txt";
    } 
    if (P==0.25) {
        if (jj==1) OutFile << "Cabs h2o " << Ti << " K Y05 P025.txt";
        else OutFile << "Cabs h2o " << Ti << " K Y " << Yi << " P025.txt";
    } 
    if (P==0.5) {
        if (jj==1) OutFile << "Cabs h2o " << Ti << " K Y05 P05.txt";
        else OutFile << "Cabs h2o " << Ti << " K Y " << Yi << " P05.txt";
    } 
    if (P>0.6) {
        if (jj==1) OutFile << "Cabs h2o " << Ti << " K Y05 P " << Pi << " .txt";
        else OutFile << "Cabs h2o " << Ti << " K Y " << Yi << " P "
                   << Pi << " .txt";
    }

    // Loop through HITEMP 2010 files (in 160 character format) and select lines
    TLN=0;

    // Loop through HITEMP2010 files
for (i=0; i<34; i++) {
    if (i==0) filein="h2o 0-50.txt";
    if (i==1) filein="h2o 50-150.txt";
    if (i==2) filein="h2o 150-250.txt";
    if (i==3) filein="h2o 250-350.txt";
    if (i==4) filein="h2o 350-500.txt";
    if (i==5) filein="h2o 500-600.txt";
    if (i==6) filein="h2o 600-700.txt";
    if (i==7) filein="h2o 700-800.txt";
    if (i==8) filein="h2o 800-900.txt";
    if (i==9) filein="h2o 900-1000.txt";
    if (i==10) filein="h2o 1000-1150.txt";
    if (i==11) filein="h2o 1150-1300.txt";
    if (i==12) filein="h2o 1300-1500.txt";
    if (i==13) filein="h2o 1500-1750.txt";
    if (i==14) filein="h2o 1750-2000.txt";
    if (i==15) filein="h2o 2000-2250.txt";
    if (i==16) filein="h2o 2250-2500.txt";
    if (i==17) filein="h2o 2500-2750.txt";
    if (i==18) filein="h2o 2750-3000.txt";
    if (i==19) filein="h2o 3000-3250.txt";
    if (i==20) filein="h2o 3250-3500.txt";
    if (i==21) filein="h2o 3500-4150.txt";
    if (i==22) filein="h2o 4150-4500.txt";
    if (i==23) filein="h2o 4500-5000.txt";
    if (i==24) filein="h2o 5000-5500.txt";
    if (i==25) filein="h2o 5500-6000.txt";
    if (i==26) filein="h2o 6000-6500.txt";
    if (i==27) filein="h2o 6500-7000.txt";
    if (i==28) filein="h2o 7000-7500.txt";
    if (i==29) filein="h2o 7500-8000.txt";
    if (i==30) filein="h2o 8000-8500.txt";
    if (i==31) filein="h2o 8500-9000.txt";
    if (i==32) filein="h2o 9000-11000.txt";
    if (i==33) filein="h2o 11000-30000.txt";

    inFile.open(filein.c_str());

    // Loop through file and extract all needed data
    while (inFile.good()) {
        inFile.ignore(14);
        inFile >> Eta >> s;
        inFile.ignore(11);
        inFile >> gammaair >> gammaself >> E >> n >> delta;
        inFile.ignore(101);

        // Shift eta for pressure effects
        Eta=Eta+delta*P;

        // Shift line intensity to temperature of interest
        s=s*Q*(exp(-c2*E/T)) / (exp(-c2*E/Tref))*(1-exp(-c2*Eta/T))
            / (1-exp(-c2*Eta/Tref));

        if (s>cutoff) {
            // Further processing or output
        }
    }
}
eta[TLN]=Eta;
S[TLN]=s;

// Collision broadened half-width
gamma[TLN]=pow((Tref/T),n)*P*(gammaair*(1-Y[jj])
+gammaself*Y[jj]);

// Doppler broadened half-width - from Modest pg 299
gamma_D[TLN]=eta[TLN]/299792458*sqrt(2*1.3807e-23*T
*0.693147181/2.99151e-26);

TLN++;

if (TLN>=currentsize) {
    currentsize=currentsize+500000;
    eta.resize(currentsize);
    S.resize(currentsize);
    gamma.resize(currentsize);
    gamma_D.resize(currentsize);
}

} // end loop for a given file

inFile.close();

} // end looping through files

//=====================================================
// Set up domain

NG=(etahigh-etalow)/dx+1;
vector<double> x(NG), C(NG);
x[0]=etalow;
for (i=1; i<NG; i++)
    x[i]=x[i-1]+dx;

//=====================================================// Apply line model

// Initialize absorption cross-section
for (i=0; i<NG; i++)
    C[i]=1e-50;

for (j=0; j<TLN; j++) {
    // Find starting point
    check=0;
    i=0;
    while (check<1) {
        if (x[i]>eta[j]) check=10;
        if (i==NG-1) check=10;
    }

    // Additional code...
}
i++; 
}

i--;  
ii=i;

// Move to the right from line center  
check=0;  
while (check<1) {

    piece=0;
    deta=abs(x[i]-eta[j]);
    voigt(S[j], gamma[j], gamma_D[j], deta, piece);

    C[i]=C[i]+piece;
    if (piece<cutoff2) check=10;
    if (deta>(cutgamma*gamma[j])) check=10;
    if (i==NG-1) check=10;

    i++;  
}

// Move to the left from line center  
check=0;  
i=ii-1;  
while (check<1) {

    piece=0;
    deta=abs(x[i]-eta[j]);
    voigt(S[j], gamma[j], gamma_D[j], deta, piece);

    C[i]=C[i]+piece;
    if (piece<cutoff2) check=10;
    if (deta>(cutgamma*gamma[j])) check=10;
    if (i==0) check=10;

    i--;  
}

//=======================================================
// Write data to a file
ofstream fileout;  
fileout.open(OutFile.str().c_str());

for (i=0; i<NG; i++)  
    fileout << x[i] << " " << C[i] << endl;

fileout.close();

cout << "Done." << endl << endl;
double partition(double T)
{
    int i;
    double Q;
    vector<double> QQ(28), TT(28);


    locate(TT, 27, T, i);

    Q=QQ[i]+(QQ[i+1]-QQ[i])*(T-TT[i])/(TT[i+1]-TT[i]);

    return Q;
}

void voigt(double& s, double& bl, double& bd, double deta, double& keta)
{
    complex<double> Z;
}

// Computes absorption coefficient for a Voigt line using the subroutine
// INPUT:
//    S    line intensity (cm^-2)
//    BL   lorentz halfwidth at halfheight (cm^-1)
//    BD   doppler halfwidth at halfheight (cm^-1)
//    DETA wavenumbers away from line center (cm^-1)
// OUTPUT:
//    KETA spectral absorption coefficient at a wavenumber deta removed
//          from line center (cm^-1)
double W, bd2;

if (bd<1e-10) bd=1e-10; // Doppler halfwidth at 1/e height (cm-1)
bd2=bd/0.8325546; // corrected BD

Z=complex<double> (deta/bd2, bl/bd2);
W=WWW(Z);
keta=s/(1.772454*bd2)*W;
}

double WWW(complex<double> Z)
{
    complex<double> W4, T, U;
    double W, X, Y, S;
    X=real(Z);
    Y=imag(Z);
    T=complex<double> (Y,-X);
    S=abs(X)+Y;
    if (S>=15.0)
        W4=T*0.5641896/(0.5+T*T);
    else if (S>=5.5) {
        U=T*T;
        W4=T*(1.410474+U*0.5641896)/(0.75+U*(3.0+U));
    }
    else if (Y>=0.195*abs(X)-.176)
    else {
        U=T*T;
        W4=exp(U)-T*(36183.31-U*(3321.9905-U*(1540.787-U*(219.0313
        -U*(35.76683-U*(1.320522-U*.5642236))))))/(32066.6-U*(24322.84
        -U*(9022.228-U*(2186.181-U*(364.2191-U*(61.57037-U*(1.841439-
        U)))))));
    }
    W=real(W4);
    return W;
}

void locate(vector<double>& xx, int n, double x, int& j) {
    unsigned long ju, jm, jl;
    int ascnd;
    jl=0;
    ju=n+1;
    // This function searches data using bisection. Adapted
    // from Recipes in C. xx is vector to search, n is max
    // index, x is value to search for, and j is lower index
    // of the two points x is between (j is the solution).
ascnd=(xx[n] >= xx[1]);
while (ju-jl>1) {
    jm=(ju+jl) >> 1;
    if (x >= xx[jm] == ascnd)
        jl=jm;
    else
        ju=jm;
}
if (x == xx[0]) j=0;
else if (x==xx[n]) j=n-1;
else j=jl;
}
APPENDIX B. LINE-BY-LINE ALBDF CODE

The code, written in C++, used to calculate the line-by-line absorption line blackbody distribution function, following the development in Section 4.1, is given here. The code shown here computes the ALBDF for a series of absorption cross-sections at the conditions specified.

// This program calculates the ALBDF for a specific case
// John Pearson
// May 3, 2011

#include<iostream>
#include<math.h>
#include<cmath>
#include<fstream>
#include<vector>
#include<string>
using namespace std;

int main()
{

    // Variable Declaration
    double T, Tg, Tb, Y, Cmin, Cmax, cav, Eb_T, ii, eta2;
    int i, j, N, NG;
    string filein;

    Tg=2500; // K (gas temperature)
    Tb=1000; // K (blackbody source temperature)
    Y=0; // mole fraction of H2O, CO2, or CO
    N=100; // number of steps in C

    // Specify file containing LBL absorption cross-section data to input
    filein=".\Cabs Data\Cabs h2o 2500K Y0 P1.txt"

    Cmin=(1e-4)/6.022045e19;
    Cmax=(60)/6.022045e19;

    vector<double> F(N), Cref(N), Eb2(22000);

    for (i=0; i<N; i++) {

\( ii = i; \)
\[
C_{ref}[i] = C_{min} \cdot \text{pow}((C_{max}/C_{min}), (ii/(N-1))); // \text{logarithmically spaced}
\]

//===============================================================================================
// Calculate values for absorption cross-section

for (i=0; i<22000; i++) Eb2[i] = 0; //Initialize

NG=0;

ifstream inFile;
string line;

inFile.open(filein.c_str());

// Count number of datapoints in file
while (inFile.good()) {
    getline(inFile,line);
    NG=NG+1;
}
NG--;

inFile.close(); // Close and reopen file to start from beginning
inFile.open(filein.c_str());

vector<double> eta(NG), C(NG);

for (i=0; i<NG; i++)
    inFile >> eta[i] >> C[i];

// Correct eta data - does not record enough significant digits
eta[0] = 0;
for (i=1; i<NG; i++)
    eta[i] = eta[i-1] + .005;

//=================================================================
// Calculate the Planck emissive power within each segment

T=Tb;
vector<double> Eb(NG);

for (i=2; i<NG; i++) {
    Eb[i] = ((3.741771e-8 * pow(eta[i], 3)) / (exp(1.43877516 * eta[i]/T) - 1) + (3.741771e-8 * pow(eta[i-1], 3)) / (exp(1.43877516 * eta[i-1]/T) - 1)) / 2;
}

eta2 = eta[NG-1] + 1;
i = 0;
while (eta2<30000) {
    i++;
    eta2++;
    Eb2[i] = ((3.741771e-8 * pow(eta2, 3)) / (exp(1.43877516 * eta2/T) - 1) + (3.741771e-8 * pow((eta2-1), 3)) / (exp(1.43877516 * (eta2-1)/T) - 1)) / 2;
Eb_T=5.6704e-8*pow(T,4); // total blackbody emissive power

//=================================================================
// Loop through spectrum
for (i=0; i<N; i++) {
    F[i]=0;
    for (j=2; j<NG; j++) {
        cav=(C[j]+C[j-1])/2;
        if (cav<Cref[i])
            F[i]=F[i]+Eb[j]*(eta[j]-eta[j-1]);
    }
    for (j=0; j<22000; j++)
        F[i]=F[i]+Eb2[j];
    F[i]=F[i]/Eb_T;
}

//=================================================================
// Write data to a file
ofstream fileout;
fileout.open("ALBDF_Calculation.out");
for (i=0; i<N; i++) {
    fileout << Cref[i] << "  " << F[i] << endl;
    // fileout << F[i] << endl;
}
fileout.close();
return(0);
APPENDIX C. CODE FOR EFFICIENT CALCULATION OF THE ALBDF

The code, written in C++, used to calculate the absorption line blackbody distribution function based on either the correlation or using tabulated data, following the development in Chapter 5, is given here. The code shown here computes the ALBDF for a series of absorption cross-sections for given conditions.

```c++
//=============================================================
// Uses the correlation and tabulated data to compute the ALBDF
// of a single gas for given conditions.
// John Pearson
// September 3, 2013

#include<iostream>
#include<math.h>
#include<cmath>
#include<fstream>
#include<vector>
#include<string>
using namespace std;

// Functions
void data_read(vector<double>& Fdata1, vector<double>& Fdata2, int molecule, int P1);
double TABLE(double Cabs, double Tg, double Tb, double Y, double P, int P1, int molecule, vector<double>& C, vector<double>& Fdata1, vector<double>& Fdata2);
void locate(vector<double>& xx, int n, double x, int& j);
double ALBDF(double Cabs, double Tg, double Tb, double Y, double P, int molecule);

int main()
{
    // Variable declarations
    double Tg, Tb, P, Y, Cmin, Cmax, ii;
    int P1, i, j, N, NG, molecule;
```
// Conditions
Tg=1508; // K (gas temperature)
Tb=2050; // K (blackbody source temperature)
P=3; // atm (total pressure)
Y=0.5; // mole fraction of H2O, CO2, or CO (in air)
molecule=1; // 1 for h2o, 2 for co2, 3 for co
N=100; // number of steps in C at which to solve for F

vector<double> F_corr(N), F_table(N), Cabs(N), Fdata1(2), Fdata2(2),
Ctab(71), PPP(10);

// max and min supplemental cross-section
Cmin=1e-4; // m2/mole
Cmax=1000; // m2/mole (value too high if using the correlation for CO)

// Set up supplemental absorption cross-section data
for (i=0; i<N; i++) {
   ii=i;
   Cabs[i]=Cmin*pow((Cmax/Cmin),(ii/(N-1)));
}

// Set up absorption cross-sections needed for tabulated data
for (i=0; i<71; i++) {
   ii=i;
   Ctab[i]=1e-4*pow((1000/1e-4),(ii/(70)));
}

// Get index of lower pressure bound
PPP[0]=0.1; PPP[1]=0.25; PPP[2]=0.5; PPP[3]=1; PPP[4]=2;

locate(PPP,9,P,P1);
if (P1==9) P1=8;

// Read data
data_read(Fdata1,Fdata2,molecule,P1);

// Calculate ALBDF using look-up table
for (i=0; i<N; i++)
   F_table[i]=TABLE(Cabs[i], Tg, Tb, Y, P, P1, molecule, Ctab, Fdata1, Fdata2);

// Calculate ALBDF using correlation
for (i=0; i<N; i++)
   F_corr[i]=ALBDF(Cabs[i], Tg, Tb, Y, P, molecule);

// Output results
ofstream fileout;
fileout.open("ALBDF_Calculation.out");

fileout << "Cabs F_table F_correlation" << endl;
for (i=0; i<N; i++)
   fileout << Cabs[i] << " " << F_table[i] << " " << F_corr[i] << endl;

fileout.close();

return(0);
This function computes the Absorption Line Blackbody Distribution Function (ALBDF) using the correlation.

double ALBDF(double Cabs, double Tg, double Tb, double Y, double PT, int molecule)
{
    double b[64], p[64], xi, xi_p, P, P2, F;
    int i, l, m, n;
    ifstream bfile, pfile;

    // Specify Coefficients
    if (molecule==1) { // H2O
        b[0]=0.978924033; b[1]=-0.207425641; b[2]=-2.806734007;
        b[3]=1.389417761;
        b[16]=0.231177379; b[17]=-0.094605006; b[18]=0.908439931; b[19]=-0.538832358;
        b[20]=0.253813018; b[21]=2.082040478; b[22]=-4.476709604;
        b[23]=2.443789298;
        b[27]=-2.473496475;
        b[28]=0.179162546; b[29]=0.78797212; b[30]=-1.520752749;
        b[31]=0.829104247;
        b[32]=0.166909096; b[33]=-0.795281465; b[34]=0.93926916; b[35]=-0.304702655;
        b[36]=-0.669061231; b[37]=3.939405065; b[38]=-4.430494571;
        b[39]=1.196316393;
        b[40]=0.83751338; b[41]=-4.931136293; b[42]=5.02756374; b[43]=-0.976626716;
        b[44]=-0.321006927; b[45]=1.907332712; b[46]=-1.76313509;
        b[47]=0.215566922;
        b[48]=0.018988364; b[49]=-0.075587929; b[50]=0.069280395;
        b[51]=2.48E-06;
        b[52]=-0.079441343; b[53]=0.346149251; b[54]=-0.231488972;
        b[55]=-0.065735266;
        b[56]=0.096930043; b[57]=-0.404603524; b[58]=0.151771109;
        b[59]=0.17764551;
        b[60]=-0.036760921; b[61]=0.147106808; b[62]=-0.014863816;
        b[63]=-0.098469241;
    }
if (molecule==2) {  // CO2
  b[7]=0.919085662;
  b[15]=0.375314671;
  b[16]=0.052165634; b[17]=0.885000092; b[18]=-0.982474572;
  b[19]=0.375314671;
  b[20]=-0.531916205; b[21]=-2.214482516; b[22]=2.293219643;
  b[23]=-0.867071711;
  b[27]=0.600486161;
  b[28]=-0.506065247; b[29]=-0.52642387; b[30]=0.340073377; b[31]=-0.101266268;
  b[32]=0.054472216; b[33]=-0.1581808; b[34]=0.29003629; b[35]=-0.137608476;
  b[36]=-0.172336869; b[37]=0.538060901; b[38]=-0.853519053;
  b[39]=0.383655517;
  b[40]=0.233085884; b[41]=-0.702110304; b[42]=1.046918448; b[43]=-0.458832711;
  b[44]=-0.10143316; b[45]=0.29115141; b[46]=-0.424020704;
  b[47]=0.184047896;
  b[48]=0.006301556; b[49]=-0.030097135; b[50]=0.044577943; b[51]=-0.019483088;
  b[52]=-0.018227338; b[53]=0.095092466; b[54]=-0.122626495;
  b[55]=0.05015993;
  b[56]=0.020997129; b[57]=-0.109841221; b[58]=0.134896941; b[59]=-0.05405009;
  b[60]=-8.18E-03; b[61]=0.04163713; b[62]=-0.05021366;
  b[63]=0.020023722;

  p[12]=0.026838401; p[13]=-0.074737215; p[14]=0.010782536;
  p[15]=0.020039736;
if (molecule==3) { // CO
    b[0]=3.316310112; b[1]=0.273254392; b[2]=-1.035375039;
b[15]=0.4577440888; b[16]=0.427224963; b[17]=0.159347829; b[18]=-0.314631881;
b[19]=0.152076858; b[20]=-1.356291059; b[21]=0.115369369; b[22]=0.658528303; b[23]=-0.372592736;
b[24]=3.663861248; b[25]=-1.945483178; b[26]=0.377631485;
b[27]=0.08835684; b[28]=-2.530222444; b[29]=2.519532063; b[30]=-1.79410425;
b[31]=0.564326917; b[32]=0.072745637; b[33]=-0.061526669; b[34]=0.033240467; b[35]=-0.004119976;
b[36]=-0.266116052; b[37]=0.003566603; b[38]=0.127097068; b[39]=-0.066171379;
b[40]=0.704482493; b[41]=-0.253535518; b[42]=-0.009919421; b[43]=0.031869833;
b[44]=0.491444366; b[45]=0.432780135; b[46]=-0.32227219;
b[47]=0.111101186; b[48]=0.004004596; b[49]=-0.005870558; b[50]=0.004038598; b[51]=-0.000880491;
b[52]=-0.015436392; b[53]=-0.00290339; b[54]=0.010857925; b[55]=-0.005012608;
b[56]=0.042245518; b[57]=-0.007520854; b[58]=-0.007585042; b[59]=0.003917497;
b[60]=-0.029663594; b[61]=0.022352969; b[62]=-0.016590884; b[63]=0.006069374;

p[27]=1.651348405; p[28]=0.177021253; p[29]=-0.05593256; p[30]=-0.401553289;
p[31]=0.245224992; p[32]=-34.73465418; p[33]=103.8477015; p[34]=-141.729319;
p[44]=-0.466208091; p[45]=0.190251348; p[46]=0.635513731; p[47]=-0.389171949;
p[56]=3.655832622; p[57]=-3.373560674; p[58]=-0.873746551; p[59]=1.050506404;
p[60]=0.305051681; p[61]=-0.094529018; p[62]=-0.378666546; p[63]=0.219049669;
}

// Calculate pressure term
xi=log(Cabs);
xi_p=0;

// Effective pressure for H2O
if (molecule==1)
    PT=(1+8.17*Y)*PT;

i=0;
for (l=0; l<4; l++) {
    for (m=0; m<4; m++) {
        for (n=0; n<4; n++) {
            xi_p=xi_p+p[i]*pow(Tg*Tb/(2500*2500), n)*pow(xi, m)*pow(log(PT*100)/10, l+1);
        }
    }
}

// Calculate P
P=0;

150
P2=0;

if (molecule==3) {
    P2=xi_p;
    xi_p=0;
}

i=0;
for (l=0; l<4; l++) {
    for (m=0; m<4; m++) {
        for (n=0; n<4; n++) {
            P=P+b[i]*pow((Tg/2500),n)*pow((Tb/2500),m) *pow((xi-xi_p),l);
            i++;
        }
    }
}

// Calculate F
F=0.5*tanh(P-P2)+0.5;
return F;

//=======================================================
//=======================================================
// This function computes the Absorption Line Blackbody // Distribution Function (ALBDF) using tables
double TABLE(double Cabs, double Tg, double Tb, double Y, double P, int Pi, int molecule, vector<double>& C, vector<double>& Fdata1, vector<double>& Fdata2) {
    int i, j, k, l, m;
    double F;
    vector<double> T(28), Fint(16), YY(9), PP(10);

    // Put values in range if they are out of bounds
    if (Cabs<C[0]) Cabs=C[0];
    if (Cabs>C[70]) Cabs=C[70];
    if (Tg<300) Tg=300;
    if (Tg>3000) Tg=3000;
    if (Tb<300) Tb=300;
    if (Tb>3000) Tb=3000;

    // Set temperature values
    T[0]=300;
    for (i=1; i<28; i++)
        T[i]=T[i-1]+100;

    // Set pressure values
    PP[0]=0.1; PP[1]=0.25; PP[2]=0.5; PP[3]=1; PP[4]=2;

    // Find location of Tg, Tb, and C
    locate(T, 27, Tg, m);
    locate(T, 27, Tb, l);
    locate(C, 70, Cabs, k);
// H2O section
if (molecule==1) {
    YY[0]=0; YY[1]=0.05; YY[2]=0.1; YY[3]=0.2; YY[4]=0.3;
    YY[5]=0.4; YY[6]=0.6; YY[7]=0.8; YY[8]=1;
    // Find location of Y
    locate(YY, 8, Y, j);
    i=j*55664+m*1988+l*71+k;
    // Interpolate in P
    Fint[0]=Fdata1[i]+(Fdata2[i]-Fdata1[i])*(P-PP[0])/(PP[1]-PP[0]);
    Fint[1]=Fdata1[i+55664]+(Fdata2[i+55664]-Fdata1[i+55664])*(P-PP[1])/(PP[1+1]-PP[1]);
    Fint[2]=Fdata1[i+1]+(Fdata2[i+1]-Fdata1[i+1])*(P-PP[0])/(PP[1+1]-PP[0]);
    Fint[3]=Fdata1[i+55735]+(Fdata2[i+55735]-Fdata1[i+55735])*(P-PP[0])/(PP[1+1]-PP[0]);
    Fint[4]=Fdata1[i+72]+(Fdata2[i+72]-Fdata1[i+72])*(P-PP[0])/(PP[1+1]-PP[0]);
    Fint[5]=Fdata1[i+57652]+(Fdata2[i+57652]-Fdata1[i+57652])*(P-PP[0])/(PP[1+1]-PP[0]);
    Fint[6]=Fdata1[i+1988]+(Fdata2[i+1988]-Fdata1[i+1988])*(P-PP[0])/(PP[1+1]-PP[0]);
    Fint[7]=Fdata1[i+57653]+(Fdata2[i+57653]-Fdata1[i+57653])*(P-PP[0])/(PP[1+1]-PP[0]);
    // Interpolate in Y
    Fint[0]=Fint[0]+(Fint[1]-Fint[0])*(Y-YY[j])/(YY[j+1]-YY[j]);
    // Interpolate in C
    Fint[0]=Fint[0]+(Fint[1]-Fint[0])*(Cabs-C[k])/(C[k+1]-C[k]);
Fint[1]=Fint[2]+(Fint[3]-Fint[2])*(Cabs-C[k])/(C[k+1]-C[k]);
Fint[3]=Fint[6]+(Fint[7]-Fint[6])*(Cabs-C[k])/(C[k+1]-C[k]);

// Interpolate in Tb
Fint[0]=Fint[0]+(Fint[1]-Fint[0])*(Tb-T[l])/(T[l+1]-T[l]);

// Interpolate in Tg
F=Fint[0]+(Fint[1]-Fint[0])*(Tg-T[m])/(T[m+1]-T[m]);
}

// CO2 or CO section
if (molecule>1) {
  i=m*1988+l*71+k;

  // Interpolate in P
  Fint[0]=Fdata1[i]+(Fdata2[i]-Fdata1[i])*(P-PP[P1])/(PP[P1+1]-PP[P1]);
  Fint[1]=Fdata1[i+1]+(Fdata2[i+1]-Fdata1[i+1])*(P-PP[P1])/(PP[P1+1]-PP[P1]);
  Fint[2]=Fdata1[i+71]+(Fdata2[i+71]-Fdata1[i+71])*(P-PP[P1])/(PP[P1+1]-PP[P1]);
  Fint[3]=Fdata1[i+72]+(Fdata2[i+72]-Fdata1[i+72])*(P-PP[P1])/(PP[P1+1]-PP[P1]);
  Fint[6]=Fdata1[i+2059]+(Fdata2[i+2059]-Fdata1[i+2059])*(P-PP[P1])/(PP[P1+1]-PP[P1]);
  Fint[7]=Fdata1[i+2060]+(Fdata2[i+2060]-Fdata1[i+2060])*(P-PP[P1])/(PP[P1+1]-PP[P1]);

  // Interpolate in C
  Fint[0]=Fint[0]+(Fint[1]-Fint[0])*(Cabs-C[k])/(C[k+1]-C[k]);
  Fint[1]=Fint[2]+(Fint[3]-Fint[2])*(Cabs-C[k])/(C[k+1]-C[k]);
  Fint[3]=Fint[6]+(Fint[7]-Fint[6])*(Cabs-C[k])/(C[k+1]-C[k]);

  // Interpolate in Tb
  Fint[0]=Fint[0]+(Fint[1]-Fint[0])*(Tb-T[l])/(T[l+1]-T[l]);

  // Interpolate in Tg
  F=Fint[0]+(Fint[1]-Fint[0])*(Tg-T[m])/(T[m+1]-T[m]);
}

return F;
}

//===============================================
// This function reads in the data for H2O, CO2, and CO

void data_read(vector<double>& Fdata1, vector<double>& Fdata2, int molecule, int P1) {
ifstream data_F1, data_F2;

if (molecule==1) {
    // Specify file locations and names
    if (P1==0) {
        data_F1.open("C:\Codes\ALBDF\Tables\h2o_p0_1.txt");
        data_F2.open("C:\Codes\ALBDF\Tables\h2o_p0_25.txt");
    }
    if (P1==1) {
        data_F1.open("C:\Codes\ALBDF\Tables\h2o_p0_25.txt");
        data_F2.open("C:\Codes\ALBDF\Tables\h2o_p0_5.txt");
    }
    if (P1==2) {
        data_F1.open("C:\Codes\ALBDF\Tables\h2o_p0_5.txt");
        data_F2.open("C:\Codes\ALBDF\Tables\h2o_p1.txt");
    }
    if (P1==3) {
        data_F1.open("C:\Codes\ALBDF\Tables\h2o_p1.txt");
        data_F2.open("C:\Codes\ALBDF\Tables\h2o_p2.txt");
    }
    if (P1==4) {
        data_F1.open("C:\Codes\ALBDF\Tables\h2o_p2.txt");
        data_F2.open("C:\Codes\ALBDF\Tables\h2o_p4.txt");
    }
    if (P1==5) {
        data_F1.open("C:\Codes\ALBDF\Tables\h2o_p4.txt");
        data_F2.open("C:\Codes\ALBDF\Tables\h2o_p8.txt");
    }
    if (P1==6) {
        data_F1.open("C:\Codes\ALBDF\Tables\h2o_p8.txt");
        data_F2.open("C:\Codes\ALBDF\Tables\h2o_p15.txt");
    }
    if (P1==7) {
        data_F1.open("C:\Codes\ALBDF\Tables\h2o_p15.txt");
        data_F2.open("C:\Codes\ALBDF\Tables\h2o_p30.txt");
    }
    if (P1>7) {
        data_F1.open("C:\Codes\ALBDF\Tables\h2o_p30.txt");
        data_F2.open("C:\Codes\ALBDF\Tables\h2o_p50.txt");
    }
}

Fdata1.resize(500976);
Fdata2.resize(500976);
for (int i=0; i<500976; i++) {
    data_F1 >> Fdata1[i];
    data_F2 >> Fdata2[i];
}

if (molecule==2) {
    if (P1==0) {
        data_F1.open("C:\Codes\ALBDF\Tables\co2_p0_1.txt");
        data_F2.open("C:\Codes\ALBDF\Tables\co2_p0_25.txt");
    }
}
if (P1==1) {
    data_F1.open("C:\Codes\ALBDF\Tables\co2_p0_25.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co2_p0_5.txt");
}
if (P1==2) {
    data_F1.open("C:\Codes\ALBDF\Tables\co2_p0_5.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co2_p1.txt");
}
if (P1==3) {
    data_F1.open("C:\Codes\ALBDF\Tables\co2_p1.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co2_p2.txt");
}
if (P1==4) {
    data_F1.open("C:\Codes\ALBDF\Tables\co2_p2.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co2_p4.txt");
}
if (P1==5) {
    data_F1.open("C:\Codes\ALBDF\Tables\co2_p4.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co2_p8.txt");
}
if (P1==6) {
    data_F1.open("C:\Codes\ALBDF\Tables\co2_p8.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co2_p15.txt");
}
if (P1==7) {
    data_F1.open("C:\Codes\ALBDF\Tables\co2_p15.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co2_p30.txt");
}
if (P1>7) {
    data_F1.open("C:\Codes\ALBDF\Tables\co2_p30.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co2_p50.txt");
}

Fdata1.resize(55664);
data2.resize(55664);
for (int i=0; i<55664; i++) {
data_F1 >> Fdata1[i];
data_F2 >> Fdata2[i];
}
if (molecule==3) {
    if (P1==0) {
        data_F1.open("C:\Codes\ALBDF\Tables\co_p0_1.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co_p0_25.txt");
    }
    if (P1==1) {
        data_F1.open("C:\Codes\ALBDF\Tables\co_p0_25.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co_p0_5.txt");
    }
    if (P1==2) {
        data_F1.open("C:\Codes\ALBDF\Tables\co_p0_5.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co_p1.txt");
    }
    if (P1==3) {
        data_F1.open("C:\Codes\ALBDF\Tables\co_p1.txt");
    }
}
data_F2.open("C:\Codes\ALBDF\Tables\co_p2.txt");
}
if (P1==4) {
    data_F1.open("C:\Codes\ALBDF\Tables\co_p2.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co_p4.txt");
}
if (P1==5) {
    data_F1.open("C:\Codes\ALBDF\Tables\co_p4.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co_p8.txt");
}
if (P1==6) {
    data_F1.open("C:\Codes\ALBDF\Tables\co_p8.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co_p15.txt");
}
if (P1==7) {
    data_F1.open("C:\Codes\ALBDF\Tables\co_p15.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co_p30.txt");
}
if (P1>7) {
    data_F1.open("C:\Codes\ALBDF\Tables\co_p30.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co_p50.txt");
}
Fdata1.resize(55664);
Fdata2.resize(55664);
for (int i=0; i<55664; i++) {
data_F1 >> Fdata1[i];
data_F2 >> Fdata2[i];
}
data_F1.close();
data_F2.close();

//========================================================
//========================================================
// This function searches data using bisection. The code is
// an adaptation of a code from Numerical Recipes in C.
// xx is vector to search, n is max index, x is value to search
// for, and j is lower index of the two points x is between.

void locate(vector<double>& xx, int n, double x, int& j) {
    unsigned long ju, jm, j1;
    int ascnd;
    jl=0;
    ju=n+1;
    ascnd=(xx[n] >= xx[1]);
    while (j1-ju>1) {
        jm=(ju+j1) >> 1;
        if (x >= xx[jm] == ascnd)
            jl=jm;
        else
            ju=jm;
}
if (x == xx[0]) j=0;
else if (x==xx[n]) j=n-1;
else j=j1;
}
APPENDIX D. SLW CODE FOR ISOTHERMAL, HOMOGENEOUS MEDIA

The code, written in C++, used to calculate the SLW solution to the radiative transfer equation for homogeneous, isothermal media is given here. The code is configured to work using either the correlation or tabulated data, as the user specifies. The code shown here outputs the radiative flux and divergence of radiative flux for given conditions.

//=================================================================
// Applies the SLW model to solve the RTE using the
// Discrete Ordinates Method
// 1-D plane layer, isothermal
// John Pearson
// May 25, 2011

#include<iostream>
#include<cmath>
#include<time.h>
#include<math.h>
#include<fstream>
#include<string>
#include<vector>
using namespace std;

// Functions
void gauss_quadrature(int n, vector<double>& mu, vector<double>& w );
double ALBDF(double Cabs, double Tg, double Tb, double Y, double P, int molecule);
void data_read(vector<double>& Fdata1, vector<double>& Fdata2, int molecule, int P1);
double TABLE(double Cabs, double Tg, double Tb, double Y, double P, int P1, int molecule, vector<double>& C, vector<double>& Fdata1, vector<double>& Fdata2);
void locate(vector<double>& xx, int n, double x, int& j);

// Main Program
int main()
{

// User specified variables
int n, num_nodes, NGG, molecule, DF;
double XL, eps0, epsL, EPS, T, T0, TL, Cmin, Cmax, Y, P;

n=36;   // order of Gaussian quadrature
num_nodes=201; // number of nodes where solution is needed
NGG=20;  // number of gray gases

// Medium properties
T=1000;  // temperature (K)
P=15;   // total pressure (atm)
Y=0.2; // mole fraction
molecule=2;  // 1 = H2O, 2 = CO2, 3 = CO
XL=1.5;  // width of gas layer (m)

// Emissivities and temperatures of walls
esp0=0.7;
espL=0.7;
T0=300; //K
TL=300; //K

// Max and min supplemental cross-section
Cmin=1e-4; // m2/mol
Cmax=600;  // m2/mol

// Convergence requirement
EPS=1.e-16;

// ALBDF Solution method
DF=1; // 1-correlation, 2-tabulated data

// Other variables used in calculations
double dx, rho0, rhoL, E_bw0, E_bwL, sum1;
double PI, DN, delta, pdif, ndif, I_bb, dgg;
vector<double> mu(n), w(n), bb(64), cc(64);
vector<double> c_sup(NGG+1), c_abs(NGG+1), kappa(NGG+1);
vector<double> a0(NGG+1), aL(NGG+1), a(NGG+1);
vector<double> x(num_nodes), F(num_nodes), Q(num_nodes);
int j, ii, it, gg, xi, ord, P1;

// Set up discrete ordinates and weights
gauss_quadrature(n, mu, w);

// Set up domain
dx=XL/(num_nodes-1); // x-step - even spacing assumed
x[0]=0;
for (xi=1; xi<num_nodes; xi++)
    x[xi]=x[xi-1]+dx;

// Calculate absorption coefficients
supplemental cross-sections
for (gg=0; gg<NGG+1; gg++) {
    dgg=gg;
    c_sup[gg]=Cmin*pow((Cmax/Cmin),(dgg/NGG));
}

gray gas absorption cross-sections and coefficients
DN=P*12187.274/T;
kappa[0]=0;
for (gg=1; gg<NGG+1; gg++) {
    c_abs[gg]=pow(c_sup[gg]*c_sup[gg-1],.5);
    kappa[gg]=Y*DN*c_abs[gg];
}

Calculate gray gas weights
if (DF==1) {   // correlations
    a[0]=ALBD(Cmin,T,T,Y,P,molecule);
    a0[0]=ALBD(Cmin,T,T0,Y,P,molecule);
    aL[0]=ALBD(Cmin,T,TL,Y,P,molecule);
    for (gg=1; gg<NGG+1; gg++) {
        a[gg]=ALBD(c_sup[gg],T,T,Y,P,molecule)-ALBD(c_sup[gg-1],T,T,Y,P,molecule);
        a0[gg]=ALBD(c_sup[gg],T,T0,Y,P,molecule)-ALBD(c_sup[gg-1],T,T0,Y,P,molecule);
        aL[gg]=ALBD(c_sup[gg],T,TL,Y,P,molecule)-ALBD(c_sup[gg-1],T,TL,Y,P,molecule);
    }
}
if (DF==2) {   // tabulated data
    vector<double> Fdata1(2), Fdata2(2), CCC(71), PPP(10);
    double iii;
    for (int i=0; i<71; i++) {
        iii=i;
        CCC[i]=1e-4*pow((1000/1e-4),(iii/70));
    }
    // Get index of lower pressure bound
    PPP[0]=0.1; PPP[1]=0.25; PPP[2]=0.5; PPP[3]=1; PPP[4]=2;
    locate(PPP,9,P,P1);
    if (P1==9) P1=8;
    // Read data from file
    data_read(Fdata1, Fdata2, molecule, P1);
    a[0]=TABLE(Cmin,T,T,Y,P,P1,molecule,CCC,Fdata1,Fdata2);
    a0[0]=TABLE(Cmin,T,T0,Y,P,P1,molecule,CCC,Fdata1,Fdata2);
\[ a_{L[0]} = \text{TABLE}(C_{\text{min}}, T, TL, Y, P, P_1, \text{molecule}, CCC, Fdata_1, Fdata_2); \]

for (gg=1; gg<\text{NGG}+1; gg++) {
    \[ a[gg] = \text{TABLE}(c_{\sup[gg]}, T, T, Y, P, P_1, \text{molecule}, CCC, Fdata_1, Fdata_2) - \text{TABLE}(c_{\sup[gg-1]}, T, T, Y, P, P_1, \text{molecule}, CCC, Fdata_1, Fdata_2); \]
    \[ a_0[gg] = \text{TABLE}(c_{\sup[gg]}, T, T_0, Y, P, P_1, \text{molecule}, CCC, Fdata_1, Fdata_2) - \text{TABLE}(c_{\sup[gg-1]}, T, T_0, Y, P, P_1, \text{molecule}, CCC, Fdata_1, Fdata_2); \]
    \[ a_{L[gg]} = \text{TABLE}(c_{\sup[gg]}, T, TL, Y, P, P_1, \text{molecule}, CCC, Fdata_1, Fdata_2) - \text{TABLE}(c_{\sup[gg-1]}, T, TL, Y, P, P_1, \text{molecule}, CCC, Fdata_1, Fdata_2); \]
}

//======================================================
// Some calculations
PI = 4.*atan(1.);
// Reflectivities at walls
\[ \rho_0 = 1.-\eps_0; \]
\[ \rho_L = 1.-\eps_L; \]
// Emissive power at wall, blackbody intensity at interior points
\[ E_{bw0} = 5.67\times10^{-8}\times\text{pow}(T_0, 4); \]
\[ E_{bwL} = 5.67\times10^{-8}\times\text{pow}(T_L, 4); \]
\[ I_{bb} = 5.67\times10^{-8}\times\text{pow}(T, 4)/\pi; \]
//=======================================================
// Initialize intensities
typedef std::vector<double> Vec1D;
typedef std::vector<Vec1D> Vec2D;
Vec2D I_pos(num_nodes, Vec1D(n));
Vec2D I_neg(num_nodes, Vec1D(n));
Vec2D I_posold(num_nodes, Vec1D(n));
Vec2D I_negold(num_nodes, Vec1D(n));
Vec2D I_pos_total(num_nodes, Vec1D(n));
Vec2D I_neg_total(num_nodes, Vec1D(n));

for (xi=0; xi<num_nodes; xi++) {
    for (gg=0; gg<n/2; gg++) {
        I_pos_total[xi][gg]=0;
        I_neg_total[xi][gg]=0;
    }
}
//=======================================================
// Start loop solving for intensities
for (gg=0; gg<\text{NGG}+1; gg++) { // loop through gray gases
    // Initialize intensities
    for (xi=0; xi<num_nodes; xi++) {
        for (ord=0; ord<n/2; ord++) {

        }
    }
}
\begin{verbatim}
I_pos[\xi][\ord]=0;
I_neg[\xi][\ord]=0;
I_posold[\xi][\ord]=0;
I_negold[\xi][\ord]=0;
}
}
delta=10;
it=0; //iteration count
do {
    it++;
    // x-loop: positive intensities
    // Apply boundary condition at x=0
    for (\ord=0; \ord<n/2; \ord++) {
        sum1=0;
        for (\ii=0; \ii<n/2; \ii++)
            sum1=sum1+w[\ii]*mu[\ii]*I_neg[0][\ii];
        I_pos[0][\ord]=\eps0*E_bw0*a0[gg]/\PI+2*\rho0*sum1;
        if (I_pos[0][\ord]<0) {
            I_pos[0][\ord]=0;
            cout << "Negative intensity corrected 1" << endl;
        }
    }
    for (\xi=1; \xi<num_nodes; \xi++) {
        for (\ord=0; \ord<n/2; \ord++) {
            dx=x[\xi]-x[\xi-1];
            I_pos[\xi][\ord]=(mu[\ord]*I_pos[\xi-1][\ord]+dx*kappa[gg]*I_bb*a[gg])
            /(mu[\ord]+dx*kappa[gg]);
            if (I_pos[\xi][\ord]<0) {
                I_pos[\xi][\ord]=0;
                cout << "Negative intensity corrected 2" << endl;
            }
        }
    }
    // x-loop: negative intensities
    // Apply boundary condition at x=L
    for (\ord=0; \ord<n/2; \ord++) {
        sum1=0;
        for (\ii=0; \ii<n/2; \ii++)
            sum1=sum1+w[\ii]*mu[\ii]*I_pos[num_nodes-1][\ii];
    }
}
\end{verbatim}
\[ I_{\text{neg}}[\text{num nodes}-1][\text{ord}]=\varepsilon L E_{bwL} a_{L[gg]}/\pi+2 \rho L \sum_1; \]

if \((I_{\text{neg}}[\text{num nodes}-1][\text{ord}]<0)\) {
    \[ I_{\text{neg}}[\text{num nodes}-1][\text{ord}]=0; \]
    \text{cout} << "Negative intensity corrected 3" << endl;
}

for \((xi=\text{num nodes}-2; xi>-1; xi--)\) {
    for \((\text{ord}=0; \text{ord}<n/2; \text{ord}++)\) {
        \[ dx=x[xi+1]-x[xi]; \]
        \[ I_{\text{neg}}[xi][\text{ord}]=\frac{\mu[\text{ord}]*I_{\text{neg}}[xi+1][\text{ord}]+dx*kappa[gg]*I_{bb*a[gg]}}{\mu[\text{ord}]+dx*kappa[gg]}; \]
        if \((I_{\text{neg}}[xi][\text{ord}]<0)\) {
            \[ I_{\text{neg}}[xi][\text{ord}]=0; \]
            \text{cout} << "Negative intensity corrected 4" << endl;
        }
    }
}

// Check convergence
delta=0;
for \((xi=0; xi<\text{num nodes}; xi++)\) {
    for \((\text{ord}=0; \text{ord}<n/2; \text{ord}++)\) {
        \[ pdif=abs(I_{\text{pos}}[xi][\text{ord}]-I_{\text{posold}}[xi][\text{ord}]); \]
        \[ ndif=abs(I_{\text{neg}}[xi][\text{ord}]-I_{\text{negold}}[xi][\text{ord}]); \]
        if \((pdif>\delta)\) \(\delta=\text{pdif};\)
        if \((ndif>\delta)\) \(\delta=\text{ndif};\)
        \[ I_{\text{posold}}[xi][\text{ord}]=I_{\text{pos}}[xi][\text{ord}]; \]
        \[ I_{\text{negold}}[xi][\text{ord}]=I_{\text{neg}}[xi][\text{ord}]; \]
    }
}

// Break loop if too many iterations (solution didn't converge)
if \((\text{it}>500)\) {
    \text{cout} << " Failure to converge" << endl;
    break;
}

while \((\delta>\text{EPS})\);

// Sum intensities
for \((xi=0; xi<\text{num nodes}; xi++)\) {
    for \((\text{ord}=0; \text{ord}<n/2; \text{ord}++)\) {
        \[ I_{\text{pos total}}[xi][\text{ord}]=I_{\text{pos total}}[xi][\text{ord}]+I_{\text{pos}}[xi][\text{ord}]; \]
        \[ I_{\text{neg total}}[xi][\text{ord}]=I_{\text{neg total}}[xi][\text{ord}]+I_{\text{neg}}[xi][\text{ord}]; \]
    }
}

} // end spectral loop
// Calculate F (flux) and Q (divergence of flux)
for (xi=0; xi<num_nodes; xi++) {
    sum1=0;
    for (ord=0; ord<n/2; ord++)
        sum1=sum1+mu[ord]*w[ord]*(I_pos_total[xi][ord]-
        I_neg_total[xi][ord]);
    F[xi]=2*PI*sum1;
}

// Q = derivative of F
vector<double> Q1(num_nodes);
for (xi=1; xi<num_nodes-1; xi++)
    Q[xi]=-(F[xi+1]-F[xi-1])/(x[xi+1]-x[xi-1]);
Q[0]=Q[1]; Q[num_nodes-1]=Q[num_nodes-2];

// Write data to a file
ofstream fileout;
fileout.open("slw_dom.out");
for (xi=0; xi<num_nodes; xi++)
    fileout << x[xi] << " " << F[xi]/1000 << " " << Q[xi]/1000 << endl;
return(0);
} // end main body

// This function sets up ordinates and weights
void gauss_quadrature(int n, vector<double>& mu, vector<double>& w )
{
    double ns, EPS, PI, x1, x2, x3, m, xm, xi, z, zl, p1, p2, p3, pp;
    int i, j;
    ns=n;
    EPS=3.E-14;
    PI=4.*atan(1.);
    x1=-1;
    x2=1;
    m=(ns+1.)/2;
    xm=0.5*(x2+x1);
    x1=0.5*(x2-x1);
    for (i=0; i<m-1; i++) {
        // ...
\[ z = \cos(\pi \cdot ((i+1)-.25)/(ns+.5)) \]

do {
    p1 = 1.;
    p2 = 0.;

    for (j=1; j<ns+1; j++) {
        p3 = p2;
        p2 = p1;
        p1 = ((2.*j-1.)*z*p2-(j-1.)*p3)/j;
    }

    pp = n*(z*p1-p2)/(z*z-1.);
    zl = z;
    z = zl - p1/pp;
}

while (abs(z-zl)>EPS);

mu[i] = xm-xl*z;
mu[n-1-i] = xm+xl*z;

w[i] = 2.*xl/((1.-z*z)*pp*pp);
w[n-1-i] = w[i];

for (i=0; i<ns/2; i++) {
    mu[i] = mu[n/2+i];
    w[i] = w[n/2+i];
}

//=======================================================
//=======================================================
// This function computes the Absorption Line Blackbody Distribution Function (ALBDF)

double ALBDF(double Cabs, double Tg, double Tb, double Y, double PT, int molecule) {
    double b[64], p[64], xi, xi_p, P, P2, P;
    int i, l, m, n;
    ifstream bfile, pfile;

    if (molecule==1) { // H2O
        b[0] = 0.978924033; b[1] = -0.207425641; b[2] = -2.806734007;
        b[3] = 1.389417761;
    }
b[16]=0.231177379; b[17]=-0.094605006; b[18]=0.908439931; b[19]=-0.538832358;
b[20]=0.253813018; b[21]=2.082040478; b[22]=-4.476709604;
b[23]=2.443789298;
b[27]=-2.473496475;
b[28]=0.179162546; b[29]=0.78797212; b[30]=-1.520752749;
b[31]=0.829104247;
b[32]=0.166909096; b[33]=-0.094605006; b[34]=0.93926916; b[35]=-0.304702655;
b[36]=0.669061231; b[37]=3.939405065; b[38]=-4.430494571;
b[39]=1.196316933;
b[40]=0.83751338; b[41]=-4.931136293; b[42]=5.027563734; b[43]=-0.976626716;
b[44]=-0.321006927; b[45]=1.90733712; b[46]=-1.76313509;
b[47]=-0.215569222;
b[48]=0.018988364; b[49]=-0.075587929; b[50]=0.069280395;
b[51]=2.48E-06;
b[52]=0.079441343; b[53]=0.346149251; b[54]=-0.231489927;
b[55]=-0.065735266;
b[56]=0.096930043; b[57]=-0.404603524; b[58]=0.151771109;
b[59]=0.177645511;
b[60]=0.036760921; b[61]=0.147106808; b[62]=-0.014863816;
b[63]=-0.098469241;
p[12]=-0.080753; p[13]=0.42606; p[14]=-0.41713;
p[15]=0.12426;
p[28]=0.56745; p[29]=-2.6102; p[30]=2.6208; p[31]=0.807;
p[32]=49.884; p[33]=105.44; p[34]=-85.162; p[35]=22.81;
p[60]=0.57955; p[61]=-2.3468; p[62]=2.3494; p[63]=-0.72409;
}
if (molecule==2) { // CO2
b[7]=0.919085662;
b[15]=0.729684329;
b[16]=0.202156834; b[17]=0.885000092; b[18]=-0.982474572;

b[19]=0.375314671;

b[20]=-0.531916205; b[21]=-2.214482516; b[22]=2.293219643;

b[23]=-0.867071711;


b[27]=0.600486161;

b[28]=-0.506065247; b[29]=-0.52642387; b[30]=0.340073377; b[31]=-0.101266268;

b[32]=0.054472216; b[33]=-0.1581808; b[34]=0.29003629; b[35]=-0.137608476;

b[36]=0.383655517;

b[37]=0.233085885; b[38]=-0.702110304; b[39]=1.046918448; b[40]=-0.458832711;

b[41]=-0.1043316; b[42]=0.29115141; b[43]=-0.424020704;

b[47]=0.184047896;

b[48]=0.006301556; b[49]=-0.030097135; b[50]=0.044577943; b[51]=-0.019483088;

b[52]=-0.018227338; 

b[53]=0.095092466; b[54]=-0.122626495;

b[55]=0.05015993;

b[56]=0.020997129; b[57]=-0.109841221; b[58]=0.134896941; b[59]=-0.054050099;

b[60]=-8.18E-03; b[61]=0.04163713; b[62]=-0.05021366;

b[63]=0.020023722;


p[12]=0.02683401; p[13]=-0.074737215; p[14]=0.010782536;

p[15]=0.020039736;


p[23]=0.442687983;


p[27]=-0.230432069;

p[28]=-0.194708661; p[29]=0.344715216; p[30]=0.082301336; p[31]=-0.169291984;

p[32]=-90.49778524; p[33]=191.2774078; p[34]=-145.3015474;

p[35]=34.01824433;

p[36]=-10.43915684; p[37]=40.10843718; p[38]=-43.29133973;

p[39]=12.82988374;

p[40]=2.551054114; p[41]=-6.770847243; p[42]=2.075279528;

p[43]=-0.815010456;

p[44]=-0.400183431; p[45]=-0.766811133; p[46]=0.018447262;

p[47]=0.238835363;


p[56]=-1.431539415; p[57]=4.097348243; p[58]=-1.864356794;

p[59]=-0.109473928;

p[60]=-0.256915604; p[61]=0.610041193; p[62]=-0.249699442; p[63]=-0.038328249;
if (molecule==3) { // CO

    b[0]=3.316310112; b[1]=0.273254392; b[2]=-1.035375039;
    b[3]=0.473979958;
    b[11]=0.687532486;
    b[15]=0.457744088;
    b[16]=0.427224963; b[17]=0.159347829; b[18]=-0.314631881;
    b[19]=0.152076858;
    b[20]=-1.356291059; b[21]=0.115369369; b[22]=0.658528303; b[23]=-0.372592736;
    b[24]=3.663861248; b[25]=-1.945483178; b[26]=0.377631485;
    b[27]=0.088835684;
    b[31]=0.564326917;
    b[32]=0.072745637; b[33]=-0.061526669; b[34]=0.033240467; b[35]=-0.004119976;
    b[36]=-0.266116052; b[37]=0.003566603; b[38]=0.127097068; b[39]=-0.066171379;
    b[40]=-0.704482493; b[41]=-0.253535518; b[42]=-0.009919421;
    b[43]=0.031869833;
    b[44]=-0.491444366; b[45]=0.432780135; b[46]=-0.32227219;
    b[47]=0.111101168;
    b[48]=0.004004596; b[49]=-0.005870558; b[50]=0.004038598; b[51]=-0.000880491;
    b[52]=-0.015436392; b[53]=-0.00290339; b[54]=0.010857925; b[55]=-0.005012608;
    b[56]=0.042245518; b[57]=-0.007520854; b[58]=-0.00758042;
    b[59]=0.003917497;
    b[60]=-0.029663594; b[61]=0.022352969; b[62]=-0.016590884;
    b[63]=0.006069374;

    p[7]=1.063879591;
    p[12]=-0.010648303; p[13]=-0.008657971; p[14]=0.096011021;
    p[15]=-0.056109023;
    p[27]=1.651348405;
    p[28]=0.177021253; p[29]=-0.05593256; p[30]=-0.401553289;
    p[31]=0.245224992;
    p[32]=-34.73465418; p[33]=103.8477015; p[34]=-141.729319;
    p[35]=58.45442338;
    p[39]=16.9208218;
\[ p[40]=-5.547243446; p[41]=5.73298138; p[42]=1.987247698; p[43]=-2.23242013; \]
\[ p[44]=-0.666208091; p[45]=0.190251348; p[46]=0.635513731; p[47]=-0.389171949; \]
\[ p[56]=3.655832622; p[57]=-3.73560674; p[58]=-0.873746551; p[59]=1.050506404; \]
\[ p[60]=0.305051681; p[61]=-0.094529018; p[62]=0.378666546; p[63]=0.219049669; \]

// Calculate pressure term
\[ \text{x}_i=\log(C_{\text{abs}}); \]
\[ \text{x}_i_\text{p}=0; \]

// Effective pressure for H2O
if (molecule==1)
\[ \text{PT}=(1+8.17*Y)*\text{PT}; \]

\[ i=0; \]
\[ \text{for (l=0; l<4; l++) { } } \]
\[ \text{for (m=0; m<4; m++) { } } \]
\[ \text{for (n=0; n<4; n++) { } } \]
\[ \text{x}_i_\text{p}=\text{x}_i_\text{p}+p[i]*\text{pow}(Tg*Tb/(2500*2500), n)*\text{pow}(\text{x}_i, m)*\text{pow}(\log(\text{PT*100})/10, 1+l); \]
\[ i++; \]

// Calculate P
\[ \text{P}=0; \]
\[ \text{P2}=0; \]

if (molecule==3) {
\[ \text{P2}=\text{x}_i_\text{p}; \]
\[ \text{x}_i_\text{p}=0; \]
}

\[ i=0; \]
\[ \text{for (l=0; l<4; l++) { } } \]
\[ \text{for (m=0; m<4; m++) { } } \]
\[ \text{for (n=0; n<4; n++) { } } \]
\[ \text{P}=\text{P}+b[i]*\text{pow}((Tg/2500), n)*\text{pow}((Tb/2500), m)*\text{pow}((\text{x}_i-\text{x}_i_\text{p}), 1); \]
\[ i++; \]

// Calculate F
\[ \text{F}=0.5*\tanh(P-P2)+0.5; \]

return F;
double TABLE(double Cabs, double Tg, double Tb, double Y, double P, int P1, int molecule, vector<double>& C, vector<double>& Fdata1, vector<double>& Fdata2) {

    int i, j, k, l, m;
    double F;
    vector<double> T(28), Fint(16), YY(9), PP(10);

    // Put values in range if they are out of bounds
    if (Cabs<C[0]) Cabs=C[0];
    if (Cabs>C[70]) Cabs=C[70];
    if (Tg<300) Tg=300;
    if (Tg>3000) Tg=3000;
    if (Tb<300) Tb=300;
    if (Tb>3000) Tb=3000;

    // Set temperature values
    T[0]=300;
    for (i=1; i<28; i++)
        T[i]=T[i-1]+100;

    // Set pressure values
    PP[0]=0.1; PP[1]=0.25; PP[2]=0.5; PP[3]=1; PP[4]=2;

    // Find location of Tg, Tb, and C
    locate(T, 27, Tg, m);
    locate(T, 27, Tb, l);
    locate(C, 70, Cabs, k);

    // H2O section
    if (molecule==1) {
        YY[0]=0; YY[1]=0.05; YY[2]=0.1; YY[3]=0.2; YY[4]=0.3;
        YY[5]=0.4; YY[6]=0.6; YY[7]=0.8; YY[8]=1;

        // Find location of Y
        locate(YY, 8, Y, j);
        i=j*55664+m*1988+l*71+k;

        // Interpolate in P
        Fint[0]=Fdata1[i]+(Fdata2[i]-Fdata1[i])*(P-PP[P1])/(PP[P1+1]-PP[P1]);
        Fint[1]=Fdata1[i+55664]+(Fdata2[i+55664]-Fdata1[i+55664])*(P-
                    PP[P1])/(PP[P1+1]-PP[P1]);
        Fint[2]=Fdata1[i+1]+(Fdata2[i+1]-Fdata1[i+1])*(P-PP[P1])/(PP[P1+1]-
                    PP[P1]);
        Fint[3]=Fdata1[i+55665]+(Fdata2[i+55665]-Fdata1[i+55665])*(P-
                    PP[P1])/(PP[P1+1]-PP[P1]);
    }
}
Fint[4] = Fdata1[i+71] + (Fdata2[i+71] - Fdata1[i+71]) * (P - PP[1]) / (PP[1+1] - PP[1]);
Fint[5] = Fdata1[i+55735] + (Fdata2[i+55735] - Fdata1[i+55735]) * (P - PP[1]) / (PP[1+1] - PP[1]);
Fint[6] = Fdata1[i+72] + (Fdata2[i+72] - Fdata1[i+72]) * (P - PP[1]) / (PP[1+1] - PP[1]);
Fint[7] = Fdata1[i+55736] + (Fdata2[i+55736] - Fdata1[i+55736]) * (P - PP[1]) / (PP[1+1] - PP[1]);
Fint[9] = Fdata1[i+57652] + (Fdata2[i+57652] - Fdata1[i+57652]) * (P - PP[1]) / (PP[1+1] - PP[1]);
Fint[12] = Fdata1[i+2059] + (Fdata2[i+2059] - Fdata1[i+2059]) * (P - PP[1]) / (PP[1+1] - PP[1]);
Fint[13] = Fdata1[i+57723] + (Fdata2[i+57723] - Fdata1[i+57723]) * (P - PP[1]) / (PP[1+1] - PP[1]);
Fint[14] = Fdata1[i+2060] + (Fdata2[i+2060] - Fdata1[i+2060]) * (P - PP[1]) / (PP[1+1] - PP[1]);
Fint[15] = Fdata1[i+57724] + (Fdata2[i+57724] - Fdata1[i+57724]) * (P - PP[1]) / (PP[1+1] - PP[1]);

// Interpolate in Y
Fint[0] = Fint[0] + (Fint[1] - Fint[0]) * (Y - YY[j]) / (YY[j+1] - YY[j]);

// Interpolate in C
Fint[0] = Fint[0] + (Fint[1] - Fint[0]) * (Cabs - C[k]) / (C[k+1] - C[k]);

// Interpolate in Tb
Fint[0] = Fint[0] + (Fint[1] - Fint[0]) * (Tb - T[l]) / (T[l+1] - T[l]);

// Interpolate in Tg
F = Fint[0] + (Fint[1] - Fint[0]) * (Tg - T[m]) / (T[m+1] - T[m]);
}

// CO2 or CO section
if (molecule>1) {
    i = m*1988 + l*71 + k;
    // Interpolate in P
    Fint[0] = Fdata1[i] + (Fdata2[i] - Fdata1[i]) * (P - PP[1]) / (PP[1+1] - PP[1]);
\[ F_{\text{int}}[1] = \text{Fdata1}[i+1] + (\text{Fdata2}[i+1] - \text{Fdata1}[i+1]) \times \frac{(P - PP[P1])}{PP[P1+1] - PP[P1]}; \]
\[ F_{\text{int}}[2] = \text{Fdata1}[i+71] + (\text{Fdata2}[i+71] - \text{Fdata1}[i+71]) \times \frac{(P - PP[P1])}{PP[P1+1] - PP[P1]}; \]
\[ F_{\text{int}}[3] = \text{Fdata1}[i+72] + (\text{Fdata2}[i+72] - \text{Fdata1}[i+72]) \times \frac{(P - PP[P1])}{PP[P1+1] - PP[P1]}; \]
\[ F_{\text{int}}[4] = \text{Fdata1}[i+1988] + (\text{Fdata2}[i+1988] - \text{Fdata1}[i+1988]) \times \frac{(P - PP[P1])}{PP[P1+1] - PP[P1]}; \]
\[ F_{\text{int}}[5] = \text{Fdata1}[i+1989] + (\text{Fdata2}[i+1989] - \text{Fdata1}[i+1989]) \times \frac{(P - PP[P1])}{PP[P1+1] - PP[P1]}; \]
\[ F_{\text{int}}[6] = \text{Fdata1}[i+2059] + (\text{Fdata2}[i+2059] - \text{Fdata1}[i+2059]) \times \frac{(P - PP[P1])}{PP[P1+1] - PP[P1]}; \]
\[ F_{\text{int}}[7] = \text{Fdata1}[i+2060] + (\text{Fdata2}[i+2060] - \text{Fdata1}[i+2060]) \times \frac{(P - PP[P1])}{PP[P1+1] - PP[P1]}; \]

// Interpolate in C
\[ F_{\text{int}}[0] = \text{Fint}[0] + (\text{Fint}[1] - \text{Fint}[0]) \times \frac{(Cabs - C[k])}{(C[k+1] - C[k])}; \]
\[ F_{\text{int}}[1] = \text{Fint}[2] + (\text{Fint}[3] - \text{Fint}[2]) \times \frac{(Cabs - C[k])}{(C[k+1] - C[k])}; \]
\[ F_{\text{int}}[2] = \text{Fint}[4] + (\text{Fint}[5] - \text{Fint}[4]) \times \frac{(Cabs - C[k])}{(C[k+1] - C[k])}; \]
\[ F_{\text{int}}[3] = \text{Fint}[6] + (\text{Fint}[7] - \text{Fint}[6]) \times \frac{(Cabs - C[k])}{(C[k+1] - C[k])}; \]

// Interpolate in Tb
\[ F_{\text{int}}[0] = \text{Fint}[0] + (\text{Fint}[1] - \text{Fint}[0]) \times \frac{(Tb - T[l])}{(T[l+1] - T[l])}; \]
\[ F_{\text{int}}[1] = \text{Fint}[2] + (\text{Fint}[3] - \text{Fint}[2]) \times \frac{(Tb - T[l])}{(T[l+1] - T[l])}; \]

// Interpolate in Tg
\[ F = \text{Fint}[0] + (\text{Fint}[1] - \text{Fint}[0]) \times \frac{(Tg - T[m])}{(T[m+1] - T[m])}; \]

return F;
}

//========================================================
//========================================================

// This function reads in the data for H2O, CO2, and CO

void data_read(vector<double>& Fdata1, vector<double>& Fdata2, int molecule, int P1) {

ifstream data_F1, data_F2;

if (molecule==1) {

    // Specify file locations and names
    if (P1==0) {
        data_F1.open("C:\Codes\ALBDF\Tables\h2o_p0_1.txt");
        data_F2.open("C:\Codes\ALBDF\Tables\h2o_p0_25.txt");
    }
    if (P1==1) {
        data_F1.open("C:\Codes\ALBDF\Tables\h2o_p0_25.txt");
        data_F2.open("C:\Codes\ALBDF\Tables\h2o_p0_5.txt");
    }
    if (P1==2) {
        data_F1.open("C:\Codes\ALBDF\Tables\h2o_p0_5.txt");
        data_F2.open("C:\Codes\ALBDF\Tables\h2o_p1.txt");
    }
    if (P1==3) {
        data_F1.open("C:\Codes\ALBDF\Tables\h2o_p1.txt");
        data_F2.open("C:\Codes\ALBDF\Tables\h2o_p2.txt");
    }
}
data_F1.open("C:\Codes\ALBDF\Tables\h2o_p1.txt");
data_F2.open("C:\Codes\ALBDF\Tables\h2o_p2.txt");
}
if (P1==4) {
data_F1.open("C:\Codes\ALBDF\Tables\h2o_p2.txt");
data_F2.open("C:\Codes\ALBDF\Tables\h2o_p4.txt");
}
if (P1==5) {
data_F1.open("C:\Codes\ALBDF\Tables\h2o_p4.txt");
data_F2.open("C:\Codes\ALBDF\Tables\h2o_p8.txt");
}
if (P1==6) {
data_F1.open("C:\Codes\ALBDF\Tables\h2o_p8.txt");
data_F2.open("C:\Codes\ALBDF\Tables\h2o_p15.txt");
}
if (P1==7) {
data_F1.open("C:\Codes\ALBDF\Tables\h2o_p15.txt");
data_F2.open("C:\Codes\ALBDF\Tables\h2o_p30.txt");
}
if (P1>7) {
data_F1.open("C:\Codes\ALBDF\Tables\h2o_p30.txt");
data_F2.open("C:\Codes\ALBDF\Tables\h2o_p50.txt");
}
Fdata1.resize(500976);
Fdata2.resize(500976);
for (int i=0; i<500976; i++) {
data_F1 >> Fdata1[i];
data_F2 >> Fdata2[i];
}

if (molecule==2) {
    if (P1==0) {
data_F1.open("C:\Codes\ALBDF\Tables\co2_p0_1.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co2_p0_25.txt");
    }
    if (P1==1) {
data_F1.open("C:\Codes\ALBDF\Tables\co2_p0_25.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co2_p0_5.txt");
    }
    if (P1==2) {
data_F1.open("C:\Codes\ALBDF\Tables\co2_p0_5.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co2_p1.txt");
    }
    if (P1==3) {
data_F1.open("C:\Codes\ALBDF\Tables\co2_p1.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co2_p2.txt");
    }
    if (P1==4) {
data_F1.open("C:\Codes\ALBDF\Tables\co2_p2.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co2_p4.txt");
    }
    if (P1==5) {
data_F1.open("C:\Codes\ALBDF\Tables\co2_p4.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co2_p8.txt");
    }
}
if (P1==6) {
    data_F1.open("C:\Codes\ALBDF\Tables\co2_p8.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co2_p15.txt");
}
if (P1==7) {
    data_F1.open("C:\Codes\ALBDF\Tables\co2_p15.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co2_p30.txt");
}
if (P1>7) {
    data_F1.open("C:\Codes\ALBDF\Tables\co2_p30.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co2_p50.txt");
}

Fdata1.resize(55664);
Fdata2.resize(5564);
for (int i=0; i<55664; i++) {
data_F1 >> Fdata1[i];
data_F2 >> Fdata2[i];
}

if (molecule==3) {
    if (P1==0) {
        data_F1.open("C:\Codes\ALBDF\Tables\co_p0_1.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co_p0_25.txt");
    }
    if (P1==1) {
        data_F1.open("C:\Codes\ALBDF\Tables\co_p0_25.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co_p0_5.txt");
    }
    if (P1==2) {
        data_F1.open("C:\Codes\ALBDF\Tables\co_p0_5.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co_p1.txt");
    }
    if (P1==3) {
        data_F1.open("C:\Codes\ALBDF\Tables\co_p1.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co_p2.txt");
    }
    if (P1==4) {
        data_F1.open("C:\Codes\ALBDF\Tables\co_p2.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co_p4.txt");
    }
    if (P1==5) {
        data_F1.open("C:\Codes\ALBDF\Tables\co_p4.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co_p8.txt");
    }
    if (P1==6) {
        data_F1.open("C:\Codes\ALBDF\Tables\co_p8.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co_p15.txt");
    }
    if (P1==7) {
        data_F1.open("C:\Codes\ALBDF\Tables\co_p15.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co_p30.txt");
    }
    if (P1>7) {

data_F1.open("C:\Codes\ALBDF\Tables\co_p30.txt");
data_F2.open("C:\Codes\ALBDF\Tables\co_p50.txt");

Fdata1.resize(55664);
Fdata2.resize(55664);
for (int i=0; i<55664; i++) {
    data_F1 >> Fdata1[i];
    data_F2 >> Fdata2[i];
}
data_F1.close();
data_F2.close();

//========================================================
//========================================================
// This function searches data using bisection.
// xx is vector to search, n is max index, x is value to search
// for, and j is lower index of the two points x is between.

void locate(vector<double>& xx, int n, double x, int& j) {

    unsigned long ju, jm, jl;
    int ascnd;

    jl=0;
    ju=n+1;
    ascnd=(xx[n] >= xx[1]);
    while ((ju-jl)>1)  {
        jm=(ju+jl) >> 1;
        if (x >= xx[jm] == ascnd)
            jl=jm;
        else
            ju=jm;
    }
    if (x == xx[0]) j=0;
    else if (x==xx[n]) j=n-1;
    else j=jl;
}
The code, written in C++, used to calculate the SLW solution to the radiative transfer equation for non-homogeneous, non-isothermal media is given here. The reference approach and multiplication method are applied. The code is configured to work using either the correlation or tabulated data, as the user specifies. The code shown here outputs the radiative flux and divergence of radiative flux for given conditions.

```cpp
// Solves RTE for non-homogeneous, non-isothermal media
// using the reference approach. Mixture of gases allowed.
// Currently configured for constant pressure systems only.
// John Pearson
// March 21, 2013

#include<iostream>
#include<math.h>
#include<cmath>
#include<time.h>
#include<fstream>
#include<vector>
#include<string>
using namespace std;

void gauss_quadrature(int n, vector<double>& mu, vector<double>& w);

double TABLE(double Cabs, double Tg, double Tb, double Y, double P,
              int P1, int molecule, vector<double>& C, vector<double>& Fdata1,
              vector<double>& Fdata2);

double ALBDF(double Cabs, double Tg, double Tb, double Y, double PT,
             int molecule);

double FMIX_TABLE(double C, double Tg, double Tb, double Y_h2o,
                   double Y_co2, double Y_co, double fv_soot, double c_soot,
                   double P, int P1, vector<double>& Ctab,
                   vector<double>& Fdataa, vector<double>& Fdatab,
                   vector<double>& Fdata2a, vector<double>& Fdata2b,
                   vector<double>& Fdata3a, vector<double>& Fdata3b);
```
double FMIX_CORR(double C, double Tg, double Tb, double Y_h2o, double Y_co2, double Y_co, double fv_soot, double c_soot, double P);
double I_ALBDP_TAB(double Fref, double Tloc, double Tref, double Y_h2o, double Y_co2, double Y_co, double fv_soot, double c_soot, double F, int P1, vector<double>& Ctab, vector<double>& Fdataa, vector<double>& Fdatab, vector<double>& Fdata2a, vector<double>& Fdata2b, vector<double>& Fdata3a, vector<double>& Fdata3b);
double I_ALBDP_COR(double Fref, double Tref, double Tloc, double Y_h2o, double Y_co2, double Y_co, double fv_soot, double c_soot, double P);
void data_read(vector<double>& Fdata1, vector<double>& Fdata2, int molecule, int P1);
void locate(vector<double>& xx, int n, double x, int& j);
double bbfn(double X);

//=========================================================
// Define parameters for case
n=36; // order of Gaussian quadrature
XL=0.8; // width of layer in meters
num_nodes=201; // number of nodes where solution is needed
NGG=20; // number of gray gases
P=1; // total pressure (atm)
vector<double> T(num_nodes), Y_h2o(num_nodes), x(num_nodes);
vector<double> Y_co2(num_nodes), Y_co(num_nodes), PPP(10);
vector<double> w(n), mu(n), Cref(NGG+1), Ctab(71);
vector<double> Fdataa(1), Fdata2a(1), Fdata3a(1), a0(NGG+1);
vector<double> Fdata2b(1), Fdata2b(1), Fdata3b(1), aL(NGG+1);
vector<double> F(num_nodes), Q(num_nodes), fv_soot(num_nodes);

// Discretize x-axis and angles
dx=XL/(num_nodes-1); // even spacing
x[0]=0;
for (xi=1; xi<num_nodes; xi++)
  x[xi]=x[xi-1]+dx;

gauss_quadrature(n, mu, w);
PI=4.*atan(1.);

// Use temperature, concentration data from file
vector<double> Bx(125), BT(125), BH2O(125), BCO2(125), BCO(125);
ifstream inFile;
inFile.open("data.txt");
B=-1;
while (inFile.good())
{
    B++;
}
inFile.close();

// Medium temperature and composition
for (i=0; i<num_nodes; i++) {
    locate(Bx, B, x[i], j);
    T[i]=BT[j]+(BT[j+1]-BT[j])*(x[i]-Bx[j])/(Bx[j+1]-Bx[j]);
    Y_h2o[i]=BH2O[j]+(BH2O[j+1]-BH2O[j])*(x[i]-Bx[j])/(Bx[j+1]-Bx[j]);
    Y_co2[i]=BCO2[j]+(BCO2[j+1]-BCO2[j])*(x[i]-Bx[j])/(Bx[j+1]-Bx[j]);
    Y_co[i]=BCO[j]+(BCO[j+1]-BCO[j])*(x[i]-Bx[j])/(Bx[j+1]-Bx[j]);
    /* // Stepwise distribution
    if (x[i]<=0.35) {
        T[i]=1000;
        Y_h2o[i]=0.2;
        Y_co2[i]=0.1;
        Y_co[i]=0.03;
    }
    if (x[i]>0.35) {
        if (x[i]<0.65) {
            T[i]=1500;
            Y_h2o[i]=0.4;
            Y_co2[i]=0.2;
            Y_co[i]=0.06;
        }
        if (x[i]>=0.65) {
            T[i]=1000;
            Y_h2o[i]=0.2;
            Y_co2[i]=0.1;
            Y_co[i]=0.03;
        }
    }
    */
    // Other distribution options
    T[i]=1000+250*cos(PI*x[i]/XL);
    T[i]=1500-1000*sin(PI*x[i]/XL);
    T[i]=985;
    Y_h2o[i]=sin(PI*x[i]/XL);
    Y_h2o[i]=0.136143;
    Y_co2[i]=0.838331;
    Y_co[i]=0;
    /*
    // soot volume fraction = soot concentration / soot density
    fv_soot[i]=0; // common values: 1e-8 < fv < 1e-5
    */
}
// Wall properties
eps0=0.8;
epsL=0.8;
T0=300;
TL=300;

// ALBDF calculation method: 1-lookup table, 2-correlation
method=1;

// Max and min supplemental cross-section
if (method==1) {
    Cmin=1e-4;
    Cmax=1000;
} else {
    Cmin=1e-4;
    Cmax=60;
}

// Soot modeling constant = 7 for arbitrary fuel, other values
// found in literature (Solovjov 2001 for example) (4.9 for propane)
c_soot=4.9;

// Convergence requirement
EPS=1.e-16;

// Set up more vectors
typedef std::vector<double> Vec1D;
typedef std::vector<Vec1D> Vec2D;

Vec2D Cloc(NGG+1,Vec1D(num_nodes));
Vec2D kappa(NGG+1,Vec1D(num_nodes));
Vec2D a(NGG+1,Vec1D(num_nodes));
Vec2D I_pos(num_nodes,Vec1D(n));
Vec2D I_neg(num_nodes,Vec1D(n));
Vec2D I_posold(num_nodes,Vec1D(n));
Vec2D I_negold(num_nodes,Vec1D(n));
Vec2D I_pos_total(num_nodes,Vec1D(n));
Vec2D I_neg_total(num_nodes,Vec1D(n));

//=========================================================  
// Choose reference state
Tref=0; Y_h2o_ref=0;
Y_co2_ref=0; Y_co_ref=0;
fv_ref=0;

// Volumetric averaging
for (i=1; i<num_nodes; i++) {
    dx=(x[i]-x[i-1])/XL;
    Tref=Tref+(T[i]+T[i-1])/2*dx;
    Y_h2o_ref=Y_h2o_ref+(Y_h2o[i]+Y_h2o[i-1])/2*dx;
    Y_co2_ref=Y_co2_ref+(Y_co2[i]+Y_co2[i-1])/2*dx;
    Y_co_ref=Y_co_ref+(Y_co[i]+Y_co[i-1])/2*dx;
    fv_ref=fv_ref+(fv_soot[i]+fv_soot[i-1])/2*dx;
}
// Can include Pref in averaging if needed
Pref=P;

//=========================================================
// Choose reference set of supplemental cross-sections
for (i=0; i<NGG+1; i++) {
    ii=i;
    Cref[i]=Cmin*exp(Cmax/Cmin, ii/NGG);
}

//=========================================================
// Calculate local set of supplemental cross-sections

// Using tables
if (method==1) {
    for (i=0; i<71; i++) {
        ii=i;
        Ctab[i]=1e-4*exp(1000/1e-4, ii/70);
    }

    // Get index of lower pressure bound
    PPP[0]=0.1; PPP[1]=0.25; PPP[2]=0.5; PPP[3]=1; PPP[4]=2;

    locate(PPP, 9, P, P1);
    if (P1==9) P1=8;

    data_read(Fdata1a, Fdata1b, 1, P1); //H2O data
    data_read(Fdata2a, Fdata2b, 2, P1); //CO2 data
    data_read(Fdata3a, Fdata3b, 3, P1); //CO data

    for (i=0; i<NGG+1; i++) {
        Fref=FMIX_TABLE(Cref[i], Tref, Tref, Y_h2o_ref, Y_co2_ref,
                         Y_co_ref, fv_ref, c_soot, Pref, P1, Ctab, Fdata1a,
                         Fdata1b, Fdata2a, Fdata2b, Fdata3a, Fdata3b);

        for (j=0; j<num_nodes; j++)
            Cloc[i][j]=I_ALBDF_TAB(Fref, T[j], Tref, Y_h2o[j],
                                   Y_co2[j], Y_co[j], fv_soot[j], c_soot, P, P1, Ctab,
                                   Fdata1a, Fdata1b, Fdata2a, Fdata2b, Fdata3a,
                                   Fdata3b);
    }
}

// Using correlations
if (method==2) {
    for (i=0; i<NGG+1; i++) {
        Fref=FMIX_CORR(Cref[i], Tref, Tref, Y_h2o_ref, Y_co2_ref,
Y_co_ref, fv_ref, c_soot, Pref);

for (j=0; j<num_nodes; j++)
    Cloc[i][j]=I_ALBDF_COR(Fref, Tref, T[j], Y_h2o[j],
                            Y_co2[j], Y_co[j], fv_soot[j], c_soot, P);
}
}

//=========================================================  
// Calculate absorption coefficients
//=========================================================  
for (j=0; j<num_nodes; j++) {
    DN=P*12187.274/T[j];
    kappa[0][j]=0;
    for (i=1; i<NGG+1; i++) {
        kappa[i][j]=DN*pow((Cloc[i][j])
                            *(Cloc[i-1][j]),.5);
    }
}

//=========================================================  
// Calculate gray-gas weights
//=========================================================  
// Using tables
if (method==1) {
    a0[0]=FMIX_TABLE(Cref[0], Tref, T0, Y_h2o_ref, Y_co2_ref,
                      Y_co_ref, fv_ref, c_soot, P, P1, Ctab, Fdata1a, Fdata1b,
                      Fdata2a, Fdata2b, Fdata3a, Fdata3b);
    aL[0]=FMIX_TABLE(Cref[0], Tref, TL, Y_h2o_ref, Y_co2_ref,
                      Y_co_ref, fv_ref, c_soot, P, P1, Ctab, Fdata1a, Fdata1b,
                      Fdata2a, Fdata2b, Fdata3a, Fdata3b);
    for (i=1; i<NGG+1; i++) {
        a0[i]=FMIX_TABLE(Cref[i], Tref, T0, Y_h2o_ref, Y_co2_ref,
                          Y_co_ref, fv_ref, c_soot, P, P1, Ctab, Fdata1a, Fdata1b,
                          Fdata2a, Fdata2b, Fdata3a, Fdata3b)
                              -FMIX_TABLE(Cref[i-1], Tref, T0, Y_h2o_ref, Y_co2_ref,
                                          Y_co_ref, fv_ref, c_soot, P, P1, Ctab, Fdata1a, Fdata1b,
                                          Fdata2a, Fdata2b, Fdata3a, Fdata3b);
        aL[i]=FMIX_TABLE(Cref[i], Tref, TL, Y_h2o_ref, Y_co2_ref,
                         Y_co_ref, fv_ref, c_soot, P, P1, Ctab, Fdata1a, Fdata1b,
                         Fdata2a, Fdata2b, Fdata3a, Fdata3b)
                              -FMIX_TABLE(Cref[i-1], Tref, TL, Y_h2o_ref, Y_co2_ref,
                                          Y_co_ref, fv_ref, c_soot, P, P1, Ctab, Fdata1a, Fdata1b,
                                          Fdata2a, Fdata2b, Fdata3a, Fdata3b);
    }
}

for (j=0; j<num_nodes; j++) {
    a[0][j]=FMIX_TABLE(Cref[0], Tref, T[j], Y_h2o_ref,
                        Y_co2_ref, Y_co_ref, fv_ref, c_soot, P, P1, Ctab,
                        Fdata1a, Fdata1b, Fdata2a, Fdata2b, Fdata3a, Fdata3b);
for (i=1; i<NGG+1; i++) {
    a[i][j]=FMIX_TABLE(Cref[i], Tref, T[j], Y_h2o_ref, Y_co2_ref, Y_co_ref, fv_ref, c_soot, P, P1, Ctab, Fdata1a, Fdata1b, Fdata2a, Fdata2b, Fdata3a, Fdata3b) - FMIX_TABLE(Cref[i-1], Tref, T[j], Y_h2o_ref, Y_co2_ref, Y_co_ref, fv_ref, c_soot, P, P1, Ctab, Fdata1a, Fdata1b, Fdata2a, Fdata2b, Fdata3a, Fdata3b);
}

// Using correlations
if (method==2) {
    a0[0]=FMIX_CORR(Cmin, Tref, T0, Y_h2o_ref, Y_co2_ref, Y_co_ref, fv_ref, c_soot, P);
    aL[0]=FMIX_CORR(Cmin, Tref, TL, Y_h2o_ref, Y_co2_ref, Y_co_ref, fv_ref, c_soot, P);
    for (i=1; i<NGG+1; i++) {
        a0[i]=FMIX_CORR(Cref[i], Tref, T0, Y_h2o_ref, Y_co2_ref, Y_co_ref, fv_ref, c_soot, P) - FMIX_CORR(Cref[i-1], Tref, T0, Y_h2o_ref, Y_co2_ref, Y_co_ref, fv_ref, c_soot, P);
        aL[i]=FMIX_CORR(Cref[i], Tref, TL, Y_h2o_ref, Y_co2_ref, Y_co_ref, fv_ref, c_soot, P) - FMIX_CORR(Cref[i-1], Tref, TL, Y_h2o_ref, Y_co2_ref, Y_co_ref, fv_ref, c_soot, P);
    }
}

for (j=0; j<num_nodes; j++) {
    a[0][j]=FMIX_CORR(Cmin, Tref, T[j], Y_h2o_ref, Y_co2_ref, Y_co_ref, fv_ref, c_soot, P);
    for (i=1; i<NGG+1; i++) {
        a[i][j]=FMIX_CORR(Cref[i], Tref, T[j], Y_h2o_ref, Y_co2_ref, Y_co_ref, fv_ref, c_soot, P) - FMIX_CORR(Cref[i-1], Tref, T[j], Y_h2o_ref, Y_co2_ref, Y_co_ref, fv_ref, c_soot, P);
    }
}

//=========================================================
// Solve RTE
// Some calculations
rho0=1.-eps0;   // Reflectivities at walls
rhoL=1.-epsL;
// Wall emissive powers
E_bw0=5.67e-8*pow(T0,4);
E_bwL=5.67e-8*pow(TL,4);

// Initialize intensities
for (xi=0; xi<num_nodes; xi++) {
    for (ord=0; ord<n/2; ord++) {
        I_pos_total[xi][ord]=0;
        I_neg_total[xi][ord]=0;
    }
}

// Start loop solving for intensities
for (gg=0; gg<NGG+1; gg++) {   // loop through gray gases

    // Initialize intensities
    for (xi=0; xi<num_nodes; xi++) {
        for (ord=0; ord<n/2; ord++) {
            I_pos[xi][ord]=0;
            I_neg[xi][ord]=0;
            I_posold[xi][ord]=0;
            I_negold[xi][ord]=0;
        }
    }

    delta=10;
    it=0;   //iteration count
    do {
        it++;

        // x-loop: positive intensities
        // Apply boundary condition at x=0
        for (ord=0; ord<n/2; ord++) {
            sum1=0;
            for (i=0; i<n/2; i++)
                sum1=sum1+w[i]*mu[i]*I_neg[0][i];
            I_pos[0][ord]=eps0*E_bw0*a0[gg]/PI+2*rho0*sum1;
            if (I_pos[0][ord]<0) {
                I_pos[0][ord]=0;
                cout << "Negative intensity corrected 1" << endl;
            }
        }

        for (xi=1; xi<num_nodes; xi++) {
            dx=x[xi]-x[xi-1];
            I_bb=5.67e-8*pow(T[xi],4)/PI;
            for (ord=0; ord<n/2; ord++) {

I_pos[xi][ord]=(mu[ord]*I_pos[xi-1][ord]+dx*kappa[gg][xi]
*I_bb*a[gg][xi])/(mu[ord]+dx*kappa[gg][xi]);
if (I_pos[xi][ord]<0) {
    I_pos[xi][ord]=0;
    cout << "Negative intensity corrected 2" << endl;
}

// x-loop: negative intensities
// Apply boundary condition at x=L
for (ord=0; ord<n/2; ord++) {
    sum1=0;
    for (i=0; i<n/2; i++)
        sum1=sum1+w[i]*mu[i]*I_pos[num_nodes-1][i];
    I_neg[num_nodes-1][ord]=epsL*E_bwL*aL[gg]/PI+2*rhoL*sum1;
    if (I_neg[num_nodes-1][ord]<0) {
        I_neg[num_nodes-1][ord]=0;
        cout << "Negative intensity corrected 3" << endl;
    }
}
for (xi=num_nodes-2; xi>-1; xi--) {
    dx=x[xi+1]-x[xi];
    I_bb=5.67e-8*pow(T[xi],4)/PI;
    for (ord=0; ord<n/2; ord++) {
        I_neg[xi][ord]=(mu[ord]*I_neg[xi+1][ord]+dx*kappa[gg][xi]
*I_bb*a[gg][xi])/(mu[ord]+dx*kappa[gg][xi]);
        if (I_neg[xi][ord]<0) {
            I_neg[xi][ord]=0;
            cout << "Negative intensity corrected 4" << endl;
        }
    }
}

// Check convergence
delta=0;
for (xi=0; xi<num_nodes; xi++) {
    for (ord=0; ord<n/2; ord++) {
        pdif=abs(I_pos[xi][ord]-I_posold[xi][ord]);
        ndif=abs(I_neg[xi][ord]-I_negold[xi][ord]);
        if (pdif>delta) delta=pdif;
if (ndif>delta) delta=ndif;
   I_posold[xi][ord]=I_pos[xi][ord];
   I_negold[xi][ord]=I_neg[xi][ord];
}
}

// Break loop if too many iterations (solution didn't converge)
if (it > 500) {
   cout << " Failure to converge" << endl;
   break;
}
}
while (delta > EPS);

// Sum intensities
for (xi=0; xi<num_nodes; xi++) {
   for (ord=0; ord<n/2; ord++) {
      I_pos_total[xi][ord]=I_pos_total[xi][ord]+I_pos[xi][ord];
      I_neg_total[xi][ord]=I_neg_total[xi][ord]+I_neg[xi][ord];
   }
}
} // end spectral loop

//=======================================================
// Calculate F and Q
for (xi=0; xi<num_nodes; xi++) {
   sum1=0;
   for (ord=0; ord<n/2; ord++) {
      sum1=sum1+mu[ord]*w[ord]*(I_pos_total[xi][ord]-
      I_neg_total[xi][ord]);
   }
   F[xi]=2*PI*sum1;
}

// Q = derivative of F
for (xi=1; xi<num_nodes-1; xi++)
   Q[xi]=-(F[xi+1]-F[xi-1])/(x[xi+1]-x[xi-1]);
Q[0]=Q[1];
Q[num_nodes-1]=Q[num_nodes-2];

//=======================================================
// Write data to a file
ofstream fileout;
fileout.open("slw_full.out");

// Output data header if desired
// fileout << "x(m) F(kW/m2) Q(kW/m3)" << endl;
// fileout << "x(m) I(kW/m2sr)" << endl;
for (xi=0; xi<num_nodes; xi++) {

// fileout /*<< x[xi] << " " */ << F[xi]/1000 //<< endl;
// /*<< " " /*<< Q[xi]/1000 /*<< endl;
fileout << x[xi] << " " << I_pos_total[xi][n/4]/1000 << " " << Q[xi]/1000 << endl;
}

fileout.close();

return(0);
}

//=========================================================
// This function sets up ordinates and weights

void gauss_quadrature(int n, vector<double>& mu, vector<double>& w )
{

double ns, EPS, PI, x1, x2, x3, m, xm, xl, z, z1, p1, p2, p3, pp;
int i, j;

ns=n;
EPS=3.E-14;
PI=4.*atan(1.);
x1=-1;
x2=1;
m=(ns+1.)/2;
xm=0.5*(x2+x1);
xl=0.5*(x2-x1);

for (i=0; i<m-1; i++) {
  z=cos(PI*((i+1)-.25)/(ns+.5));
  do {
    p1=1.;
    p2=0.;
    for (j=1; j<ns+1; j++) {
      p3=p2;
      p2=p1;
      p1=((2.*j-1.)*z*p2-(j-1.)*p3)/j;
    }
    pp=n*(z*p1-p2)/(z*z-1.);
    z1=z;
    z=z1-p1/pp;
  } while (abs(z-z1)>EPS);

  mu[i]=xm-xl*z;
  mu[n-1-i]=xm+xl*z;
  
}
\[ w[i] = 2 \cdot x_l / ((1 - z \cdot z) \cdot pp \cdot pp); \]
\[ w[n-1-i] = w[i]; \]

for (i=0; i<ns/2; i++) {
    mu[i] = mu[n/2+i];
    w[i] = w[n/2+i];
}

// These functions invert the ALBDF to obtain local values
// of absorption cross-section.

double I_ALBDF_TAB(double Fref, double Tloc, double Tref,
    double Y_h2o, double Y_co2, double Y_co, double fv_soot,
    double c_soot, double P, int P1, vector<double>& Ctab,
    vector<double>& Fdata1a, vector<double>& Fdata1b,
    vector<double>& Fdata2a, vector<double>& Fdata2b,
    vector<double>& Fdata3a, vector<double>& Fdata3b)
{
    double C1, C2, expC1, expC2, Cloc, tol, step, F1, F2, diff;
    int check, it;
    C1 = -1;
    step = 1;
    tol = 1e-6;
    check = 0;
    it = 0;
    // if Fref=1, then move to .999 to make sure look-up table works
    if (Fref > 0.999) Fref = 0.999;
    while (check < 1) {
        it++;
        C2 = C1 + step;
        if (C2 < -9.2103404) C2 = -9.2103404;
        if (C2 > 6.9077553) C2 = 6.9077553;
        expC1 = exp(C1);
        expC2 = exp(C2);
        F1 = FMIX_TABLE(expC1, Tloc, Tref, Y_h2o, Y_co2, Y_co,
            fv_soot, c_soot, P, P1, Ctab, Fdata1a, Fdata1b,
            Fdata2a, Fdata2b, Fdata3a, Fdata3b);
        F2 = FMIX_TABLE(expC2, Tloc, Tref, Y_h2o, Y_co2, Y_co,
            fv_soot, c_soot, P, P1, Ctab, Fdata1a, Fdata1b,
            Fdata2a, Fdata2b, Fdata3a, Fdata3b);
        if (it == 1) {
            if (F1 > Fref) step = -step;
        }
    }
// Check convergence
diff=abs(F1-Fref);
if (diff<tol) {
    Cloc=C2;
    check=10;
}

// Case where moving down to data point
if (F1>Fref) {
    // data point between F1 and F2
    if (F2<Fref) step=step/2; // decrease step size, try again

    // data point below both F1 and F2
    if (F2>Fref) {
        if (F2<F1) C1=C2; // move lower
    }

    // if you hit a local minimum in the correlation
    if (F2>=F1) {
        step=step/2;
        if (abs(step)<tol) {
            Cloc=C1;
            check=10;
        }
    }

    // if you reach the bottom of the look-up table
    if (C2<=-9.2103404) {
        if (C1<=-9.2103404) {
            Cloc=C1;
            check=10;
        }
    }
}

// Case where moving up to data point
if (F1<Fref) {
    // data point between F1 and F2
    if (F2<Fref) step=step/2; // decrease step size, try again

    // data point above both F1 and F2
    if (F2>Fref) {
        if (F2>F1) C1=C2; // move higher
    }

    // if you hit a maximum in the correlation (less than 1)
    if (F2<=F1) {
        step=step/2;
        if (abs(step)<tol) {
            Cloc=C1;
            check=10;
        }
    }
}
// if you reach the top of the look-up table
if (C2>=6.9077553) {
    if (C1>=6.9077553) {
        Cloc=C1;
        check=10;
    }
}
}
}
return exp(Cloc);
}

double I_ALBDF_COR(double Fref, double Tref, double Tloc,
    double Y_h2o, double Y_co2, double Y_co, double fv_soot,
    double c_soot, double P)
{
    double tol, C1, C2, expC1, expC2, Cloc, step, F1, F2, diff;
    int check, it;

    // if Fref=1, then move to .999
    if (Fref>0.999) Fref=0.999;

    C1=-1;
    step=0.5;
    tol=1e-6;

    check=0;
    it=0;

    while (check<1) {
        it++;
        C2=C1+step;
        expC1=exp(C1);
        expC2=exp(C2);

        F1=FMIX_CORR(expC1, Tloc, Tref, Y_h2o, Y_co2, Y_co,
            fv_soot, c_soot, P);
        F2=FMIX_CORR(expC2, Tloc, Tref, Y_h2o, Y_co2, Y_co,
            fv_soot, c_soot, P);

        if (it==1) {
            if (F1>Fref) step=-step;
        }

        // Check convergence
        diff=abs(F2-Fref);
        if (diff<tol) {
            Cloc=C2;
            check=10;
        }
    }
}

189
// Case where moving down to data point
if (F1>Fref) {
    // data point between F1 and F2
    if (F2<Fref) step=step/2; // decrease step size, try again

    // data point below both F1 and F2
    if (F2>Fref) {
        if (F2<F1) C1=C2; // move lower
    }

    // if you hit a local minimum in the correlation
    if (F2>=F1) {
        step=step/2;

        if (abs(step)<tol) {
            Cloc=C1;
            check=10;
        }
    }
}

// Case where moving up to data point
if (F1<Fref) {
    // data point between F1 and F2
    if (F2<Fref) step=step/2; // decrease step size, try again

    // data point above both F1 and F2
    if (F2>Fref) {
        if (F2>F1) C1=C2; // move higher
    }

    // if you hit a maximum in the correlation (less than 1)
    if (F2<=F1) {
        step=step/2;

        if (abs(step)<tol) {
            Cloc=C1;
            check=10;
        }
    }
}

return exp(Cloc);

//==================================================================
// These functions calculate the ALBDF for mixtures of gases.

double FMIX_TABLE(double C, double Tg, double Tb, double Y_h2o,
    double Y_co2, double Y_co, double fv_soot, double c_soot,
    double P, int P1, vector<double>& Ctab,
    vector<double>& Fdata1a, vector<double>& Fdata1b,
    vector<double>& Fdata2a, vector<double>& Fdata2b,
vector<double>& Fdata3a, vector<double>& Fdata3b)
{
  double Fmix, t;
  // initialize
  Fmix=1;

  if (Y_h2o>0)
    Fmix=Fmix*TABLE(C/Y_h2o,Tg,Tb,Y_h2o,P,P1,1,Ctab,Fdata1a,Fdata1b);

  if (Y_co2>0)
    Fmix=Fmix*TABLE(C/Y_co2,Tg,Tb,1,P,P1,2,Ctab,Fdata2a,Fdata2b);

  if (Y_co>0)
    Fmix=Fmix*TABLE(C/Y_co,Tg,Tb,1,P,P1,3,Ctab,Fdata3a,Fdata3b);

  if (fv_soot>0)
    Fmix=Fmix*bbfn(C*P*7.3392315e23/(100*c_soot*fv_soot*Tg*Tb*6.022045e19));

  return Fmix;
}

double FMIX_CORR(double C, double Tg, double Tb, double Y_h2o,
  double Y_co2, double Y_co, double fv_soot, double c_soot, double P)
{
  double Fmix, t;
  // initialize
  Fmix=1;

  if (Y_h2o>0)
    Fmix=Fmix*ALBDF(C/Y_h2o,Tg,Tb,Y_h2o,P,1);

  if (Y_co2>0)
    Fmix=Fmix*ALBDF(C/Y_co2,Tg,Tb,1,P,2);

  if (Y_co>0)
    Fmix=Fmix*ALBDF(C/Y_co,Tg,Tb,1,P,3);

  if (fv_soot>0)
    Fmix=Fmix*bbfn(C*P*7.3392315e23/(100*c_soot*fv_soot*Tg*Tb*6.022045e19));

  return Fmix;
}

//================================================================
// This function computes the Absorption Line Blackbody
// Distribution Function (ALBDF) using tables

191
double TABLE(double Cabs, double Tg, double Tb, double Y, double P, int P1, int molecule, vector<double>& C, vector<double>& Fdata1, vector<double>& Fdata2) {

    int i, j, k, l, m;
    double F;
    vector<double> T(28), Fint(16), YY(9), PP(10);

    // Put values in range if they are out of bounds
    if (Cabs<C[0]) Cabs=C[0];
    if (Cabs>C[70]) Cabs=C[70];
    if (Tg<300) Tg=300;
    if (Tg>3000) Tg=3000;
    if (Tb<300) Tb=300;
    if (Tb>3000) Tb=3000;

    // Set temperature values
    T[0]=300;
    for (i=1; i<28; i++)
        T[i]=T[i-1]+100;

    // Set pressure values
    PP[0]=0.1; PP[1]=0.25; PP[2]=0.5; PP[3]=1; PP[4]=2;

    // Find location of Tg, Tb, and C
    locate(T, 27, Tg, m);
    locate(T, 27, Tb, l);
    locate(C, 70, Cabs, k);

    // H2O section
    if (molecule==1) {

        YY[0]=0; YY[1]=0.05; YY[2]=0.1; YY[3]=0.2; YY[4]=0.3;
        YY[5]=0.4; YY[6]=0.6; YY[7]=0.8; YY[8]=1;

        // Find location of Y
        locate(YY, 8, Y, j);

        i=j*55664+m*1988+l*71+k;

        // Interpolate in P
        Fint[0]=Fdata1[i]+(Fdata2[i]-Fdata1[i])*(P-PP[P1])/(PP[P1+1]-PP[P1]);
        Fint[1]=Fdata1[i+55664]+(Fdata2[i+55664]-Fdata1[i+55664])*(P-PP[P1])/(PP[P1+1]-PP[P1]);
        Fint[2]=Fdata1[i+1]+(Fdata2[i+1]-Fdata1[i+1])*(P-PP[P1])/(PP[P1+1]-PP[P1]);
        Fint[3]=Fdata1[i+55665]+(Fdata2[i+55665]-Fdata1[i+55665])*(P-PP[P1])/(PP[P1+1]-PP[P1]);
        Fint[4]=Fdata1[i+71]+(Fdata2[i+71]-Fdata1[i+71])*(P-PP[P1])/(PP[P1+1]-PP[P1]);
        Fint[5]=Fdata1[i+55735]+(Fdata2[i+55735]-Fdata1[i+55735])*(P-PP[P1])/(PP[P1+1]-PP[P1]);
        Fint[6]=Fdata1[i+72]+(Fdata2[i+72]-Fdata1[i+72])*(P-PP[P1])/(PP[P1+1]-PP[P1]);
        Fint[7]=Fdata1[i+55736]+(Fdata2[i+55736]-Fdata1[i+55736])*(P-PP[P1])/(PP[P1+1]-PP[P1]);
    }
}
\[ F_{\text{int}[8]} = F_{\text{data1}[i+1988]} + (F_{\text{data2}[i+1988]} - F_{\text{data1}[i+1988]}) \frac{(P - PP[P1])}{(PP[P1+1] - PP[P1])}; \]
\[ F_{\text{int}[9]} = F_{\text{data1}[i+57652]} + (F_{\text{data2}[i+57652]} - F_{\text{data1}[i+57652]}) \frac{(P - PP[P1])}{(PP[P1+1] - PP[P1])}; \]
\[ F_{\text{int}[10]} = F_{\text{data1}[i+1989]} + (F_{\text{data2}[i+1989]} - F_{\text{data1}[i+1989]}) \frac{(P - PP[P1])}{(PP[P1+1] - PP[P1])}; \]
\[ F_{\text{int}[11]} = F_{\text{data1}[i+57653]} + (F_{\text{data2}[i+57653]} - F_{\text{data1}[i+57653]}) \frac{(P - PP[P1])}{(PP[P1+1] - PP[P1])}; \]
\[ F_{\text{int}[12]} = F_{\text{data1}[i+2059]} + (F_{\text{data2}[i+2059]} - F_{\text{data1}[i+2059]}) \frac{(P - PP[P1])}{(PP[P1+1] - PP[P1])}; \]
\[ F_{\text{int}[13]} = F_{\text{data1}[i+57723]} + (F_{\text{data2}[i+57723]} - F_{\text{data1}[i+57723]}) \frac{(P - PP[P1])}{(PP[P1+1] - PP[P1])}; \]
\[ F_{\text{int}[14]} = F_{\text{data1}[i+2060]} + (F_{\text{data2}[i+2060]} - F_{\text{data1}[i+2060]}) \frac{(P - PP[P1])}{(PP[P1+1] - PP[P1])}; \]
\[ F_{\text{int}[15]} = F_{\text{data1}[i+57724]} + (F_{\text{data2}[i+57724]} - F_{\text{data1}[i+57724]}) \frac{(P - PP[P1])}{(PP[P1+1] - PP[P1])}; \]

// Interpolate in Y
Fint[0] = Fint[0] + (Fint[1] - Fint[0]) \frac{(Y - YY[j])}{(YY[j+1] - YY[j])};

// Interpolate in C
Fint[0] = Fint[0] + (Fint[1] - Fint[0]) \frac{(\text{Cabs} - C[k])}{(C[k+1] - C[k])};

// Interpolate in Tb
Fint[0] = Fint[0] + (Fint[1] - Fint[0]) (Tb - T[l]) / (T[l+1] - T[l]);

// Interpolate in Tg
P = Fint[0] + (Fint[1] - Fint[0]) (Tg - T[m]) / (T[m+1] - T[m]);
}

// CO2 or CO section
if (molecule>1) {
    i = m*1988 + l*71 + k;

    // Interpolate in P
    Fint[0] = Fdata1[i] + (Fdata2[i] - Fdata1[i]) * (P - PP[P1]) / (PP[P1+1] - PP[P1]);
    Fint[1] = Fdata1[i+1] + (Fdata2[i+1] - Fdata1[i+1]) * (P - PP[P1]) / (PP[P1+1] - PP[P1]);
    Fint[2] = Fdata1[i+71] + (Fdata2[i+71] - Fdata1[i+71]) * (P - PP[P1]) / (PP[P1+1] - PP[P1]);
    Fint[3] = Fdata1[i+72] + (Fdata2[i+72] - Fdata1[i+72]) * (P - PP[P1]) / (PP[P1+1] - PP[P1]);
}
\[
F_{\text{int}5} = F_{\text{data1}[i+1989]} + (F_{\text{data2}[i+1989]} - F_{\text{data1}[i+1989]}) \times \frac{(P - P_{P1})}{(P_{P1+1} - P_{P1})};
\]
\[
F_{\text{int}6} = F_{\text{data1}[i+2059]} + (F_{\text{data2}[i+2059]} - F_{\text{data1}[i+2059]}) \times \frac{(P - P_{P1})}{(P_{P1+1} - P_{P1})};
\]
\[
F_{\text{int}7} = F_{\text{data1}[i+2060]} + (F_{\text{data2}[i+2060]} - F_{\text{data1}[i+2060]}) \times \frac{(P - P_{P1})}{(P_{P1+1} - P_{P1})};
\]

// Interpolate in C
\[
F_{\text{int}0} = F_{\text{int}0} + (F_{\text{int}1} - F_{\text{int}0}) \times \frac{(\text{Cabs} - C_{k})}{(C_{k+1} - C_{k})};
\]
\[
F_{\text{int}1} = F_{\text{int}2} + (F_{\text{int}3} - F_{\text{int}2}) \times \frac{(\text{Cabs} - C_{k})}{(C_{k+1} - C_{k})};
\]
\[
F_{\text{int}2} = F_{\text{int}4} + (F_{\text{int}5} - F_{\text{int}4}) \times \frac{(\text{Cabs} - C_{k})}{(C_{k+1} - C_{k})};
\]
\[
F_{\text{int}3} = F_{\text{int}6} + (F_{\text{int}7} - F_{\text{int}6}) \times \frac{(\text{Cabs} - C_{k})}{(C_{k+1} - C_{k})};
\]

// Interpolate in T_{b}
\[
F_{\text{int}0} = F_{\text{int}0} + (F_{\text{int}1} - F_{\text{int}0}) \times \frac{(T_{b} - T_{l})}{(T_{l+1} - T_{l})};
\]
\[
F_{\text{int}1} = F_{\text{int}2} + (F_{\text{int}3} - F_{\text{int}2}) \times \frac{(T_{b} - T_{l})}{(T_{l+1} - T_{l})};
\]

// Interpolate in T_{g}
\[
F = F_{\text{int}0} + (F_{\text{int}1} - F_{\text{int}0}) \times \frac{(T_{g} - T_{m})}{(T_{m+1} - T_{m})};
\]

return F;
}

//========================================================
//========================================================
// This function reads in the data for H2O, CO2, and CO
void data_read(vector<double>& Fdata1, vector<double>& Fdata2, int molecule, int P1) {

ifstream data_F1, data_F2;

if (molecule==1) {
    // Specify file locations and names
    if (P1==0) {
        data_F1.open("C:\Codes\ALBDF\Tables\h2o_p0_1.txt");
        data_F2.open("C:\Codes\ALBDF\Tables\h2o_p0_25.txt");
    }
    if (P1==1) {
        data_F1.open("C:\Codes\ALBDF\Tables\h2o_p0_25.txt");
        data_F2.open("C:\Codes\ALBDF\Tables\h2o_p0_5.txt");
    }
    if (P1==2) {
        data_F1.open("C:\Codes\ALBDF\Tables\h2o_p0_5.txt");
        data_F2.open("C:\Codes\ALBDF\Tables\h2o_p1.txt");
    }
    if (P1==3) {
        data_F1.open("C:\Codes\ALBDF\Tables\h2o_p1.txt");
        data_F2.open("C:\Codes\ALBDF\Tables\h2o_p2.txt");
    }
    if (P1==4) {
        data_F1.open("C:\Codes\ALBDF\Tables\h2o_p2.txt");
        data_F2.open("C:\Codes\ALBDF\Tables\h2o_p4.txt");
    }
    if (P1==5) {
}
data_F1.open("C:\\Codes\\ALBDF\\Tables\\h2o_p4.txt");
data_F2.open("C:\\Codes\\ALBDF\\Tables\\h2o_p8.txt");
}
if (P1==6) {
data_F1.open("C:\\Codes\\ALBDF\\Tables\\h2o_p8.txt");
data_F2.open("C:\\Codes\\ALBDF\\Tables\\h2o_p15.txt");
}
if (P1==7) {
data_F1.open("C:\\Codes\\ALBDF\\Tables\\h2o_p15.txt");
data_F2.open("C:\\Codes\\ALBDF\\Tables\\h2o_p30.txt");
}
if (P1>7) {
data_F1.open("C:\\Codes\\ALBDF\\Tables\\h2o_p30.txt");
data_F2.open("C:\\Codes\\ALBDF\\Tables\\h2o_p50.txt");
}
Fdata1.resize(500976);
Fdata2.resize(500976);
for (int i=0; i<500976; i++) {
data_F1 >> Fdata1[i];
data_F2 >> Fdata2[i];
}
}
if (molecule==2) {
if (P1==0) {
data_F1.open("C:\\Codes\\ALBDF\\Tables\\co2_p0_1.txt");
data_F2.open("C:\\Codes\\ALBDF\\Tables\\co2_p0_25.txt");
}
if (P1==1) {
data_F1.open("C:\\Codes\\ALBDF\\Tables\\co2_p0_25.txt");
data_F2.open("C:\\Codes\\ALBDF\\Tables\\co2_p0_5.txt");
}
if (P1==2) {
data_F1.open("C:\\Codes\\ALBDF\\Tables\\co2_p0_5.txt");
data_F2.open("C:\\Codes\\ALBDF\\Tables\\co2_p1.txt");
}
if (P1==3) {
data_F1.open("C:\\Codes\\ALBDF\\Tables\\co2_p1.txt");
data_F2.open("C:\\Codes\\ALBDF\\Tables\\co2_p2.txt");
}
if (P1==4) {
data_F1.open("C:\\Codes\\ALBDF\\Tables\\co2_p2.txt");
data_F2.open("C:\\Codes\\ALBDF\\Tables\\co2_p4.txt");
}
if (P1==5) {
data_F1.open("C:\\Codes\\ALBDF\\Tables\\co2_p4.txt");
data_F2.open("C:\\Codes\\ALBDF\\Tables\\co2_p8.txt");
}
if (P1==6) {
data_F1.open("C:\\Codes\\ALBDF\\Tables\\co2_p8.txt");
data_F2.open("C:\\Codes\\ALBDF\\Tables\\co2_p15.txt");
}
if (P1==7) {
data_F1.open("C:\\Codes\\ALBDF\\Tables\\co2_p15.txt");
data_F2.open("C:\\Codes\\ALBDF\\Tables\\co2_p30.txt");
}
if (P1>7) {
    data_F1.open("C:\\Codes\\ALBDF\\Tables\\co2_p30.txt");
    data_F2.open("C:\\Codes\\ALBDF\\Tables\\co2_p50.txt");
}

Fdata1.resize(55664);
Fdata2.resize(55664);
for (int i=0; i<55664; i++) {
    data_F1 >> Fdata1[i];
    data_F2 >> Fdata2[i];
}

if (molecule==3) {
    if (P1==0) {
        data_F1.open("C:\\Codes\\ALBDF\\Tables\\co_p0_1.txt");
        data_F2.open("C:\\Codes\\ALBDF\\Tables\\co_p0_25.txt");
    }
    else if (P1==1) {
        data_F1.open("C:\\Codes\\ALBDF\\Tables\\co_p0_25.txt");
        data_F2.open("C:\\Codes\\ALBDF\\Tables\\co_p0_5.txt");
    }
    else if (P1==2) {
        data_F1.open("C:\\Codes\\ALBDF\\Tables\\co_p0_5.txt");
        data_F2.open("C:\\Codes\\ALBDF\\Tables\\co_p1.txt");
    }
    else if (P1==3) {
        data_F1.open("C:\\Codes\\ALBDF\\Tables\\co_p1.txt");
        data_F2.open("C:\\Codes\\ALBDF\\Tables\\co_p2.txt");
    }
    else if (P1==4) {
        data_F1.open("C:\\Codes\\ALBDF\\Tables\\co_p2.txt");
        data_F2.open("C:\\Codes\\ALBDF\\Tables\\co_p4.txt");
    }
    else if (P1==5) {
        data_F1.open("C:\\Codes\\ALBDF\\Tables\\co_p4.txt");
        data_F2.open("C:\\Codes\\ALBDF\\Tables\\co_p8.txt");
    }
    else if (P1==6) {
        data_F1.open("C:\\Codes\\ALBDF\\Tables\\co_p8.txt");
        data_F2.open("C:\\Codes\\ALBDF\\Tables\\co_p15.txt");
    }
    else if (P1==7) {
        data_F1.open("C:\\Codes\\ALBDF\\Tables\\co_p15.txt");
        data_F2.open("C:\\Codes\\ALBDF\\Tables\\co_p30.txt");
    }
    else if (P1>7) {
        data_F1.open("C:\\Codes\\ALBDF\\Tables\\co_p30.txt");
        data_F2.open("C:\\Codes\\ALBDF\\Tables\\co_p50.txt");
    }
}

Fdata1.resize(55664);
Fdata2.resize(55664);
for (int i=0; i<55664; i++) {
    data_F1 >> Fdata1[i];
void locate(vector<double>& xx, int n, double x, int& j) {
    unsigned long ju, jm, jl;
    int ascnd;
    jl=0;
    ju=n+1;
    ascnd=(xx[n] >= xx[1]);
    while (ju-jl>1) {
        jm=(ju+jl) >> 1;
        if (x >= xx[jm] == ascnd)
            jl=jm;
        else
            ju=jm;
    }
    if (x == xx[0]) j=0;
    else if (x==xx[n]) j=n-1;
    else j=jl;
}

double ALBDF(double Cabs, double Tg, double Tb, double Y, double PT, int molecule)
{
    double b[64], p[64], xi, xi_p, P, P2, F;
    int i, l, m, n;
    ifstream bfile, pfile;
    if (molecule==1) { // H2O
    }
4.203825171;
b[16]=0.231177379; b[17]=-0.94605006; b[18]=0.908439931; b[19]=
-0.538832358;
b[20]=0.253813018; b[21]=2.082040478; b[22]=-4.76709604;
b[23]=2.443789298;
b[27]=-2.473496475;
b[28]=0.179162546; b[29]=0.78797212; b[30]=1.520752749;
b[31]=0.829104247;
b[32]=0.166909096; b[33]=-0.795281465; b[34]=0.93926916; b[35]=
-0.304702655;
b[36]=-0.669061231; b[37]=3.939405065; b[38]=4.430494571;
b[39]=1.196316393;
b[40]=0.83751338; b[41]=-4.931136293; b[42]=5.02756374; b[43]=
-0.976626716;
b[44]=-0.321006927; b[45]=1.907332712; b[46]=-1.76313509;
b[47]=0.215566922;
b[48]=0.018988364; b[49]=0.075587929; b[50]=0.069280395;
b[51]=2.48E-06;
b[52]=-0.079441343; b[53]=0.346149251; b[54]=-0.231488972;
b[55]=-0.065735266;
b[56]=0.096930043; b[57]=-0.404603524; b[58]=0.151771109;
b[59]=0.17764551;
b[60]=-0.036760921; b[61]=0.147106808; b[62]=-0.014863816;
b[63]=-0.098469241;
p[12]=-0.080753; p[13]=0.42606; p[14]=-0.41713;
p[15]=0.12426;
p[28]=0.56745; p[29]=-2.6102; p[30]=2.6208; p[31]=-0.807;
p[32]=49.884; p[33]=105.44; p[34]=-85.162; p[35]=22.81;
p[56]=3.6337; p[57]=-13.111; p[58]=8.1435; p[59]=-0.5727;
p[60]=0.57955; p[61]=-2.3468; p[62]=2.3494; p[63]=-0.72409;

if (molecule==2) {  // CO2
0.20979996;
b[7]=0.919085662;
-1.516418994;
\[ b[12]=-1.505796719; \ b[13]=0.522031728; \ b[14]=-1.653998778; \]
\[ b[15]=0.729684329; \ b[16]=0.202156834; \ b[17]=0.885000092; \ b[18]=-0.982474572; \]
\[ b[19]=0.375314671; \ b[20]=-0.531916205; \ b[21]=-2.214482516; \ b[22]=2.293219643; \]
\[ b[23]=-0.867071711; \ b[24]=1.019794785; \ b[25]=1.912899157; \ b[26]=-1.688329914; \]
\[ b[27]=0.600486161; \ b[28]=-0.506065247; \ b[29]=-0.52642387; \ b[30]=0.340073377; \]
\[ b[31]=-0.101266268; \ b[32]=0.054472216; \ b[33]=-0.1581808; \ b[34]=0.29003629; \]
\[ b[35]=-0.458832711; \ b[36]=0.172336669; \ b[37]=0.538060901; \ b[38]=-0.853519053; \]
\[ b[39]=0.383655517; \ b[40]=0.233085884; \ b[41]=-0.702110304; \ b[42]=1.046918448; \]
\[ b[43]=-0.424020704; \ b[44]=-0.10143316; \ b[45]=0.29115141; \ b[46]=-0.019483088; \]
\[ b[47]=0.006301556; \ b[48]=-0.030097135; \ b[49]=0.044577943; \ b[50]=-0.19483088; \]
\[ b[51]=0.05015993; \ b[52]=-0.018227338; \ b[53]=0.095092466; \ b[54]=-0.122626495; \]
\[ b[55]=0.05015993; \ b[56]=0.020997129; \ b[57]=-0.109841221; \ b[58]=0.134896941; \]
\[ b[59]=-0.05405009; \ b[60]=-8.18E-03; \ b[61]=0.04163713; \ b[62]=-0.05021366; \]
\[ b[63]=0.020023722; \]
\[ p[0]=-14.9838124; \ p[1]=38.41682512; \ p[2]=-37.08708237; \]
\[ p[7]=-1.65531401; \ p[8]=0.240326019; \ p[9]=-1.253645566; \ p[10]=0.926603383; \]
\[ p[11]=-0.175741918; \ p[12]=0.026838401; \ p[13]=-0.074737215; \ p[14]=0.010782536; \]
\[ p[15]=0.020039736; \ p[16]=65.6646184; \ p[17]=-153.1300705; \ p[18]=134.5182112; \]
\[ p[23]=0.442687983; \ p[24]=-1.457123086; \ p[25]=4.493581565; \ p[26]=-1.904072879; \]
\[ p[27]=-0.230432069; \ p[28]=-0.194708661; \ p[29]=0.344715216; \ p[30]=0.082301336; \]
\[ p[31]=-0.169291984; \ p[32]=-90.49778524; \ p[33]=191.2774078; \ p[34]=-145.3015474; \]
\[ p[35]=34.01824433; \ p[36]=-10.43915684; \ p[37]=40.10843718; \ p[38]=-43.29133973; \]
\[ p[39]=12.82988374; \ p[40]=2.551054114; \ p[41]=-6.770847243; \ p[42]=2.075279528; \]
\[ p[43]=0.815010456; \ p[44]=0.400183431; \ p[45]=-0.766811133; \ p[46]=0.018447262; \]
\[ p[47]=0.238853863; \ p[48]=41.94117422; \ p[49]=-79.99441926; \ p[50]=49.60377935; \]
\[ p[51]=-7.294292574; \ p[52]=7.51406621; \ p[53]=-36.3335072; \ p[54]=42.51857862; \]
\[ p[55]=-14.30274633; \ p[56]=-1.431539415; \ p[57]=4.097348243; \ p[58]=-1.864356794; \]
\[ p[59]=-0.109473928; \]
\[p[60]=-0.256915604; \ p[61]=0.610041193; \ p[62]=-0.249699442; \]
\[p[63]=-0.038328249; \]

```{if (molecule==3) { // CO}

```b[0]=3.316310112; \ b[1]=0.273254392; \ b[2]=-1.035375039; 
```
\[b[3]=0.473979958; \]
```
```
\[b[7]=-0.875343857; \]
```
\[b[8]=15.32452431; \ b[9]=-3.644252282; \ b[10]=-0.372777673; \]
```
\[b[11]=0.687532486; \]
```
```
\[b[15]=0.457744088; \]
```
\[b[16]=0.427224963; \ b[17]=0.159347829; \ b[18]=-0.314631881; \]
```
\[b[19]=0.152076858; \]
```
\[b[20]=-1.356291059; \ b[21]=0.115369369; \ b[22]=0.658528303; \ b[23]=-0.372592736; \]
```
\[b[24]=3.663861248; \ b[25]=-1.945483178; \ b[26]=0.377631485; \]
```
\[b[27]=0.088835684; \]
```
\[b[28]=-2.530222444; \ b[29]=2.519532063; \ b[30]=-1.79410425; \]
```
\[b[31]=0.564326917; \]
```
\[b[32]=0.072745637; \ b[33]=-0.061526669; \ b[34]=0.033240467; \]
```
\[b[35]=-0.004119976; \]
```
\[b[36]=-0.266116052; \ b[37]=0.003566603; \ b[38]=0.127097068; \]
```
\[b[39]=-0.066171379; \]
```
\[b[40]=0.704482493; \ b[41]=-0.253535518; \ b[42]=-0.009919421; \]
```
\[b[43]=0.031869833; \]
```
\[b[44]=0.491444366; \ b[45]=0.432780135; \ b[46]=-0.32227219; \]
```
\[b[47]=0.111101186; \]
```
\[b[48]=0.004004596; \ b[49]=-0.005870558; \ b[50]=0.004038598; \ b[51]=-0.000880491; \]
```
\[b[52]=-0.015436392; \ b[53]=-0.00290339; \ b[54]=0.010857925; \ b[55]=-0.005012608; \]
```
\[b[56]=0.042245518; \ b[57]=-0.007520854; \ b[58]=-0.007585042; \]
```
\[b[59]=0.003917497; \]
```
\[b[60]=-0.029663594; \ b[61]=0.022352969; \ b[62]=-0.016590884; \]
```
\[b[63]=0.006069374; \]
```
```
\[p[3]=4.868721547; \]
```
\[p[4]=-1.029852518; \ p[5]=5.343062546; \]
```
\[p[6]=-4.23212745; \]
```
\[p[7]=1.063879591; \]
```
\[p[8]=-0.12552327; \ p[9]=0.29017319; \]
```
\[p[10]=0.608824895; \]
```
\[p[11]=-0.457268847; \]
```
\[p[12]=-0.010648303; \]
```
\[p[13]=-0.008657971; \ p[14]=-0.096011021; \]
```
\[p[15]=-0.056109023; \]
```
\[p[16]=30.9289566; \]
```
\[p[17]=-62.58487087; \ p[18]=76.96827504; \]
```
\[p[19]=30.93824358; \]
```
\[p[20]=7.656923091; \]
```
```
\[p[23]=-8.605697097; \]
```
\[p[24]=2.104107011; \]
```
\[p[25]=-2.63598025; \]
```
\[p[26]=-1.777881616; \]
```
\[p[27]=1.651348405; \]
```
\[p[28]=0.177021253; \]
```
\[p[29]=-0.05593256; \]
```
\[p[30]=-0.401553289; \]
```
\[p[31]=0.245224992; \]
```
\[p[32]=-34.73465418; \]
```
\[p[33]=103.8477015; \]
```
\[p[34]=-141.729319; \]
```
\[p[35]=58.45442338; \]
\[ p[36]=-15.4237926; \ p[37]=49.47310879; \ p[38]=-48.57742671; \]
\[ p[39]=16.9208218; \]
\[ p[40]=-5.547243446; \ p[41]=5.732398138; \ p[42]=1.987247698; \]
\[ p[43]=-2.23242013; \]
\[ p[44]=-0.466208091; \ p[45]=0.190251348; \ p[46]=0.635513731; \]
\[ p[47]=-0.389171949; \]
\[ p[48]=11.61823155; \ p[49]=-57.78495547; \ p[50]=84.50680302; \]
\[ p[51]=-35.10802171; \]
\[ p[52]=8.766127928; \ p[53]=27.37822507; \ p[54]=28.39218696; \]
\[ p[55]=-10.34802912; \]
\[ p[56]=3.655832622; \ p[57]=-3.373560674; \ p[58]=-0.873746551; \]
\[ p[59]=1.050506404; \]
\[ p[60]=0.305051681; \ p[61]=-0.094529018; \]
\[ p[62]=-0.37866546; \]
\[ p[63]=0.219049669; \]

// Calculate pressure term
xi=log(Cabs);
xii_p=0;

// Effective pressure for H2O
if (molecule==1)
  PT=(1+8.17*Y)*PT;

i=0;
for (l=0; l<4; l++)
  for (m=0; m<4; m++)
    for (n=0; n<4; n++)
      xi_p=xi_p+p[i]*pow(Tg*Tb/(2500*2500),n)*pow(xi,m)*pow(log(PT*100)/10,l+1);
i++;

// Calculate P
P=0;
P2=0;
if (molecule==3) {
  P2=xi_p;
  xi_p=0;
}
i=0;
for (l=0; l<4; l++)
  for (m=0; m<4; m++)
    for (n=0; n<4; n++)
      P=P+b[i]*pow((Tg/2500),n)*pow((Tb/2500),m)*pow((xi-xi_p),l);
i++;

// Calculate F
F=.5*tanh(P-P2)+.5;
double bbfn(double X)
{
    double PI, CC, C2, XM, EPS, BBFN, SUM, M;
    PI=4.*atan(1.);
    CC=15/pow(PI,4);
    C2=1.43877516;  //cm*K
    EPS=1E-10;
    X=C2*X;
    M=0;
    BBFN=0;
    SUM=1;
    while (SUM>EPS) {
        M++;
        XM=X*M;
        SUM=(6-exp(-XM)*(6+XM*(6+XM*(3+XM))))/pow(M,4);
        BBFN=BBFN+SUM;
    }
    BBFN=CC*BBFN;
    return BBFN;
}
APPENDIX F. LBL CODE FOR 1-D RADIATIVE TRANSFER

The code, written in C++, used to calculate the line-by-line solution to the radiative transfer equation for the stepwise temperature and concentration profiles of Section 6.5 is given here. The code shown here outputs the radiative flux and divergence of radiative flux for given conditions. The solution for a case with a single layer instead of three is a simplification of this code and is not given.

//===-----------------------------------------------------------------===
// Solves the RTE using the line-by-line method for a case of
// non-isothermal, non-homogeneous gas layer with stepwise
// temperature and concentration distributions.
// John Pearson
// May 30, 2013
//===-----------------------------------------------------------------===
#include<iostream>
#include<cmath>
#include<math.h>
#include<fstream>
#include<string>
#include<vector>
using namespace std;

// Functions
void gauss_quadrature(int n, vector<double>& mu, vector<double>& w);

// Main Program
int main()
{

  // Variable declarations
  double XL, eps0, epsL, EPS, T0, TL;
  double Yh2o1, Yco21, Yco1, Yh2o2, Yco22, Yco2, P;
  int cc;
  string filein1, filein2, filein3, filein4, filein5, filein6;
  ofstream fileout;

  // (...)}
const int n=36; // order of Gaussian quadrature
const int num_nodes=201; // number of solution nodes

// Medium properties
vector<double> T(num_nodes), kappa(num_nodes);
P=1; // atm (total pressure)

// width of layer in m
XL=1;

// Mole fractions
Yh2o1=0.2;
Yco21=0.1;
Yco1=0.03;
Yh2o2=0.4;
Yco22=0.2;
Yco2=0.06;

// Wall properties
eps0=0.8;
epsL=0.8;
T0=1000; //K
TL=1000; //K

// convergence requirement
EPS=1.e-16;

// Specify files with absorption cross-section data to read in
filein1="Cabs h2o 1000K Y2 P1.txt";
filein2="Cabs co2 1000K P1.txt";
filein3="Cabs co 1000K P1.txt";
filein4="Cabs h2o 1500K Y4 P1.txt";
filein5="Cabs co2 1500K P1.txt";
filein6="Cabs co 1500K P1.txt";

fileout.open("mix_P1.out");

//=======================================================
// Other variables used in calculations
double PI, dx, rho0, rhoL, E_bw0, E_bwL, sum1, sum2, delta;
vector<double> mu(n), w(n), x(num_nodes), I_bb(num_nodes);
vector<double> G(num_nodes), F(num_nodes), Q(num_nodes);
double pdif, ndif, deta;
int i, j, ii, it, gg, xi, ord;

//=======================================================
// Set up domain
dx=XL/(num_nodes-1); // x-step
x[0]=0;
for (i=1; i<num_nodes; i++)
    x[i]=x[i-1]+dx;

// Specify temperature distribution
for (int i=0; i<num_nodes; i++) {
    if (x[i]<=0.35) T[i]=1000;
    if (x[i]>0.35) {
        if (x[i]<0.65) T[i]=1500;
        if (x[i]>=0.65) T[i]=1000;
    }
}

//=======================================================
// Set up discrete ordinates and weights
gauss_quadrature(n, mu, w); //call function

//=======================================================
// Some calculations
PI=4.*atan(1.0);
const int n2=n/2;

// Reflectivities at walls
rho0=1.-eps0;
rhoL=1.-epsL;

//=======================================================
// Calculate values for absorption cross-section

ifstream inFile;
string line;

// Read file 1
int NGG=0;

// Count number of points in file
inFile.open(filein1.c_str());
while (inFile.good()) {
    getline(inFile,line);
    NGG=NGG+1;
}
NGG--;
inFile.close(); // Close and reopen file to start from beginning
inFile.open(filein1.c_str());

// set up vectors
vector<double> eta(NGG), C(NGG), C1(NGG), C2(NGG);

for (i=0; i<NGG; i++) {
    inFile >> eta[i] >> C[i];
    C1[i]=C[i]*Yh2o1;
}
inFile.close();

const int NG=NGG;
// Read file 2
NGG=0;

inFile.open(filein2.c_str());
while (inFile.good()) {
    getline(inFile,line);
    NGG=NGG+1;
}
NGG--;
inFile.close(); // Close and reopen file to start from beginning
inFile.open(filein2.c_str());

for (i=0; i<NGG; i++) {
    inFile >> eta[i] >> C[i];
    C1[i]=C1[i]+C[i]*Yco21;
}
inFile.close();

// Read file 3
NGG=0;

inFile.open(filein3.c_str());
while (inFile.good()) {
    getline(inFile,line);
    NGG=NGG+1;
}
NGG--;
inFile.close(); // Close and reopen file to start from beginning
inFile.open(filein3.c_str());

for (i=0; i<NGG; i++) {
    inFile >> eta[i] >> C[i];
    C1[i]=C1[i]+C[i]*Yco1;
}
inFile.close();

// Read file 4
NGG=0;

inFile.open(filein4.c_str());
while (inFile.good()) {
    getline(inFile,line);
    NGG=NGG+1;
}
NGG--;  

inFile.close();     // Close and reopen file to start from beginning  
inFile.open(filein4.c_str());  

for (i=0; i<NGG; i++) {  
    inFile >> eta[i] >> C[i];  
    C2[i]=C[i]*Yh2o2;  
}  

inFile.close();  

// Read file 5  
NGG=0;  

inFile.open(filein5.c_str());  

while (inFile.good()) {  
    getline(inFile,line);  
    NGG=NGG+1;  
}  

NGG--;  

inFile.close();     // Close and reopen file to start from beginning  
inFile.open(filein5.c_str());  

for (i=0; i<NGG; i++) {  
    inFile >> eta[i] >> C[i];  
    C2[i]=C2[i]+C[i]*Yco22;  
}  

inFile.close();  

// Read file 6  
NGG=0;  

inFile.open(filein6.c_str());  

while (inFile.good()) {  
    getline(inFile,line);  
    NGG=NGG+1;  
}  

NGG--;  

inFile.close();     // Close and reopen file to start from beginning  
inFile.open(filein6.c_str());  

for (i=0; i<NGG; i++) {  
    inFile >> eta[i] >> C[i];  
    C2[i]=C2[i]+C[i]*Yco2;  
}  

inFile.close();
// correct eta data - files don't have enough significant digits
for (i=1; i<NG; i++)
    eta[i]=eta[i-1]+0.005;

//===----------------------------------------------------------------------===
//=== Set up vectors
//===----------------------------------------------------------------------===
typedef std::vector<double> Vec1D;
typedef std::vector<Vec1D> Vec2D;

Vec2D I_pos(num_nodes,Vec1D(n2));
Vec2D I_neg(num_nodes,Vec1D(n2));
Vec2D I_posold(num_nodes,Vec1D(n2));
Vec2D I_negold(num_nodes,Vec1D(n2));
Vec2D I_pos_total(num_nodes,Vec1D(n2));
Vec2D I_neg_total(num_nodes,Vec1D(n2));

//===----------------------------------------------------------------------===
//-- Initialize intensities
for (i=0; i<num_nodes; i++) {
    for (j=0; j<n/2; j++) {
        I_pos_total[i][j]=0;
        I_neg_total[i][j]=0;
    }
}

//===----------------------------------------------------------------------===
//-- Start loop solving for intensities
for (gg=2; gg<NG; gg++) {          // spectral loop

//===----------------------------------------------------------------------===
//-- Initialize intensities, set absorption coefficient values
for (i=0; i<num_nodes; i++) {
    for (j=0; j<n/2; j++) {
        I_pos[i][j]=0;
        I_neg[i][j]=0;
        I_negold[i][j]=0;
        I_posold[i][j]=0;
    }

    I_bb[i]=((3.741771e-8*pow(eta[gg],3))/(exp(1.43877516*eta[gg]/T[i])-1)
            +(3.741771e-8*pow(eta[gg-1],3))/(exp(1.43877516*eta[gg-1]/T[i])-1))/(2*PI);

    if (T[i]==2000) kappa[i]=P*(7.3392315e23/T[i])*(C1[gg]+C1[gg-1])/2;
    if (T[i]==3000) kappa[i]=P*(7.3392315e23/T[i])*(C2[gg]+C2[gg-1])/2;
}

E_bw0=((3.741771e-8*pow(eta[gg],3))/(exp(1.43877516*eta[gg]/T0)-1)
       +(3.741771e-8*pow(eta[gg-1],3))/(exp(1.43877516*eta[gg-1]/T0)-1))/(2*PI);

E_bwL=((3.741771e-8*pow(eta[gg],3))/(exp(1.43877516*eta[gg]/TL)-1)
       +(3.741771e-8*pow(eta[gg-1],3))/(exp(1.43877516*eta[gg-1]/TL)-1))/(2);

it=0;     //iteration counter
do {

    it++;

    // x-loop: positive intensities
    // Apply boundary condition at x=0
    for (ord=0; ord<n/2; ord++) {
        sum1=0;
        for (ii=0; ii<n/2; ii++)
            sum1=sum1+w[ii]*mu[ii]*I_neg[0][ii];
        I_pos[0][ord]=eps0*E_bw0/PI+2*rho0*sum1;
        if (I_pos[0][ord]<0) {
            I_pos[0][ord]=0;
            cout << "Negative intensity corrected" << endl;
        }
    }
    for (xi=1; xi<num_nodes; xi++) {
        dx=x[xi]-x[xi-1];
        for (ord=0; ord<n/2; ord++) {
            I_pos[xi][ord]=(mu[ord]*I_pos[xi-1][ord]+dx*kappa[xi]*I_bb[xi]) /
                           (mu[ord]+dx*kappa[xi]);
            if (I_pos[xi][ord]<0) {
                I_pos[xi][ord]=0;
                cout << "Negative intensity corrected" << endl;
            }
        }
    }

    // x-loop: negative intensities
    // Apply boundary condition at x=L
    for (ord=0; ord<n/2; ord++) {
        sum1=0;
        for (ii=0; ii<n/2; ii++)
            sum1=sum1+w[ii]*mu[ii]*I_pos[num_nodes-1][ii];
        I_neg[num_nodes-1][ord]=epsL*E_bwL/PI+2*rhoL*sum1;
        if (I_neg[num_nodes-1][ord]<0) {
            I_neg[num_nodes-1][ord]=0;
            cout << "Negative intensity corrected" << endl;
        }
    }
    for (xi=num_nodes-2; xi>-1; xi--) {
        dx=x[xi]-x[xi-1];
        for (ord=0; ord<n/2; ord++) {
            I_neg[xi][ord]=(mu[ord]*I_neg[xi+1][ord]+dx*kappa[xi]*I_bb[xi]) /
                            (mu[ord]+dx*kappa[xi]);
            if (I_neg[xi][ord]<0) {
                I_neg[xi][ord]=0;
                cout << "Negative intensity corrected" << endl;
            }
        }
    }
}
dx=x[\text{xi}+1]-x[\text{xi}];

for (ord=0; ord<n/2; ord++) {

\text{I\_neg}[\text{xi}][ord]=(\mu[ord]\times\text{I\_neg}[\text{xi}+1][ord]+dx\times\kappa[\text{xi}]\times\text{I\_bb}[\text{xi}])
\quad/(\mu[ord]+dx\times\kappa[\text{xi}]);

if (\text{I\_neg}[\text{xi}][ord]<0) {
    \text{I\_neg}[\text{xi}][ord]=0;
    cout \text{ "Negative intensity corrected" } \text{ endl;}
}
}

// Check convergence
delta=0;
for (xi=0; xi<num\_nodes; xi++) {
    for (ord=0; ord<n/2; ord++) {
        pdif=abs(I\_pos[\text{xi}][ord]-I\_posold[\text{xi}][ord]);
        ndif=abs(I\_neg[\text{xi}][ord]-I\_negold[\text{xi}][ord]);
        if (pdif>delta) delta=pdif;
        if (ndif>delta) delta=ndif;
        I\_posold[\text{xi}][ord]=I\_pos[\text{xi}][ord];
        I\_negold[\text{xi}][ord]=I\_neg[\text{xi}][ord];
    }
}

// Break loop if too many iterations (solution didn't converge)
if (\text{it} > 500) {
    cout \text{ "Failure to converge" } \text{ endl;}
    break;
}
}
while (\text{delta} > \text{EPS});
deta=\eta[gg]-\eta[gg-1];

// Sum intensities
def \text{for} (xi=0; xi<num\_nodes; xi++) {
    for (ord=0; ord<n/2; ord++) {
        I\_pos\_total[\text{xi}][ord]=I\_pos\_total[\text{xi}][ord]+I\_pos[\text{xi}][ord]\times deta;
        I\_neg\_total[\text{xi}][ord]=I\_neg\_total[\text{xi}][ord]+I\_neg[\text{xi}][ord]\times deta;
    }
}

// end spectral loop

//==============================================
// Calculate F (flux) and Q (divergence of flux)
for (i=0; i<num\_nodes; i++) {
    \text{sum2}=0;
for (j=0; j<n/2; j++)
    sum2=sum2+mu[j]*w[j]*(I_pos_total[i][j]-I_neg_total[i][j]);

    F[i]=2*PI*sum2;
}

// Q = derivative of F
vector<double> Q1(num_nodes);
for (i=1; i<num_nodes-1; i++)
    Q[i]=-(F[i+1]-F[i-1])/(x[i+1]-x[i-1]);

Q[0]=Q[1]; Q[num_nodes-1]=Q[num_nodes-2];

// Write data to a file
fileout << "x(m) F(kW/m²) Q(kW/m³)" << endl;
for (i=0; i<num_nodes; i++)
    fileout << x[i] << " " << F[i]/1000 << " " << Q[i]/1000 << endl;
fileout.close();
return(0);

} // end main body

// This function sets up ordinates and weights
void gauss_quadrature(int n, vector<double>& mu, vector<double>& w) {

double ns, EPS, PI, x1, x2, m, xm, xl;
double z, z1, p1, p2, p3, pp;
int i, j;

ns=n;
EPS=3.E-14;
PI=4.*atan(1.);

x1=-1;
x2=1;

m=(ns+1.)/2;
xm=0.5*(x2+x1);
xl=0.5*(x2-x1);

for (i=0; i<m-1; i++) {
    z=cos(PI*(((i+1)-.25)/(ns+.5)));
    do {
p1=1.;
p2=0.;

for (j=1; j<ns+1; j++) {
    p3=p2;
p2=p1;
p1=((2.*j-1.)*z*p2-(j-1.)*p3)/j;
}

pp=n*(z*p1-p2)/(z*z-1.);
z1=z;
z=z1-p1/pp;

while (abs(z-z1)>EPS);

mu[i]=xm-xl*z;
mu[n-1-i]=xm+xl*z;

w[i]=2.*xl/((1.-z*z)*pp*pp);
w[n-1-i]=w[i];

for (i=0; i<ns/2; i++) {
    mu[i]=mu[n/2+i];
w[i]=w[n/2+i];
}

}