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## A new development for the WBW model at elevated pressure levels

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### Abstract

This paper proposes an approach to obtain correlations for high pressure conditions for the weighted-sum-of-gray-gases (WSGG) model. The proposed formulation, which extends the wide-band based WSGG (WBW) model, entails solving the gray gas coefficients by partitioning the spectrum into a series of spectral intervals, and then using the classic version of the WSGG model to individually solve each segment. The line-by-line (LBL) method is used in the WBW model to first calculate the emittance of each band in which the spectra was divided. Polynomial temperature fits are then employed to compute the temperature and pressure-absorption coefficients. The sum of the contributions from every spectral band individually yields the overall radiative heat source and radiative heat flux. Showing deviations in most cases less than 5 % concerning the benchmark solution, the results demonstrate that, even at high pressures, the proposed method is capable to accurately resolve the radiative transfer.

*Keywords:* radiative transfer, participating medium, spectral models, wide-band models, high pressures

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## 1 1. Introduction

2 In combustion processes, which occur at elevated temperatures, the thermal  
3 radiation is frequently the principal mechanism of heat transfer because of  
4 the soot and participating gases formation [1]. The modeling of radiation in  
5 combustion processes under atmospheric conditions is already a very arduous  
6 task, however in scenarios at high pressure, it can become considerably more  
7 difficult [2]. Nevertheless, despite of the challenges, studies involving combustion  
8 at high pressures have recently gained attention [3–6], since strict environmental  
9 regulations, motivated by worries about global warming, urge the adoption of  
10 protocols in an effort to lessen the release of emission pollutant resulting from  
11 the burning of fossil fuels [7].

12 Rockets, gas turbines and piston engines are only a few examples of combus-  
13 tion systems that work at high pressures higher [2]. Oxy-combustion is another  
14 example of high pressure combustion, which is employed to capture and storage  
15 carbon [8]. Accurately describing the participating medium's radiative transfer is  
16 essential for optimizing combustion processes, particularly those that take place  
17 at elevated pressures, which present a higher computational cost in comparison  
18 to those that occur at atmospheric pressure. The total pressure system is also  
19 influenced by thermal radiation. As the radiation absorption rises with the  
20 total pressure and that the pressure also influences the chemical reactions, this  
21 significance increases at high pressures [9]. The increase in the soot production  
22 is the main way that soot radiation impacts the chemical reactions and is highly  
23 dependent on the pressure [2].

24 Transitions in vibrational and rotational energy states produce spectral lines  
25 centered around specific wavenumbers that are responsible for the absorption  
26 and emission of gases' thermal radiation. The generation of the properties of the  
27 gases with a high level of detail is achievable with high-resolution databases, as  
28 the HITEMP [10] and HITRAN [11], for instance. The entire radiation spectrum  
29 of gaseous species can include millions of spectral lines, each of which has its own  
30 dependence regarding the thermodynamic conditions (total pressure, temperature

31 and molar composition of the gases involved). The LBL benchmark solution  
32 [12] of the RTE, which takes into account each of these lines, allows for the  
33 calculation of thermal radiation with great accuracy. However, this methodology  
34 entails prohibitive computational costs for most real applications in engineering.  
35 Therefore, the advancements of accurate spectral models for the RTE solution is  
36 of great interest [13].

37 A great number of global spectral models, including the full-spectrum  
38 correlated- $k$  (FSCK) method [14] and the spectral line-based WSGG (SLW)  
39 model [15], were developed with the intention of fastly and accurately deter-  
40 mining the properties of the chemical species. Among them, the WSGG model  
41 [16] is the simplest, and perhaps the most widely used even as of today. In the  
42 WSGG model, the radiative intensity integration over all the wavenumbers is  
43 substituted by a sum over the partial intensities associated to each gray gas, and  
44 the erratic behavior of the spectrum of the participating medium is substituted  
45 by a little group of gray gases that occupy not necessary uninterrupted, fixed  
46 portions of the spectrum, for which the RTE is solved separately. In addition  
47 to being suitable for numerical calculations in engineering, the simplicity of the  
48 WSGG model allows it to save computational resources and ensure computational  
49 accuracy [17]. It can also be combined with computational fluid dynamics (CFD)  
50 solvers in order to resolve practical problems, having been recently applied by  
51 Refs. [18–20].

52 While atmospheric pressure conditions have generally yielded satisfactory  
53 results for the WSGG model [21–31], there are only a few applications of the  
54 model to high pressure combustion [3, 5, 32]. Since there are few WSGG correla-  
55 tions available at high pressures, some authors have attempted unsuccessfully to  
56 use these coefficients to high pressures scenarios, but they had obtained unsatis-  
57 factory results [33–35]. In high pressure situations, the WSGG coefficients are  
58 commonly applied at pressures between 1 atm and 40 atm [3, 4, 36, 37]. Above  
59 40 atm, the WSGG model was studied by [5, 6].

60 As an alternative to the radiative calculation at high pressures, Paul et. al  
61 [38] proposed a simplified stepwise-gray spectral model, under the premise that

62 the smoothing of the absorption spectrum as the total pressure increases would  
63 allow the use of a band model, which is easier to implement into code than  
64 global models. A similar band mode was developed and tested by Johnson et  
65 al. [39]. When compared to the benchmark solution, the obtained results from  
66 other spectral models, including the SLW, SNB, SNBCK and FSK, were likewise  
67 extended to high pressure scenarios and showed satisfactory accuracy. The SLW  
68 model, for instance, was applied to pressures in the range of 0.1 atm and 50 atm  
69 by Refs. [40, 41] for participating media composed of  $\text{H}_2\text{O}$ ,  $\text{CO}_2$  and  $\text{CO}$ , and  
70 for jet diffusion flames ranging from atmospheric pressure up to 30 atm by [35].  
71 The FSK method was studied at high pressures by [33–35, 42–45] providing  
72 accurate solutions. For systems subjected to total pressures over 30 atm, the  
73 SNBCK model presented maximum deviations of 2.5% in relation to the SNB  
74 model [33–35, 43].

75 The current work's purpose is to bring a formulation for the WSGG model's  
76 high-pressure coefficient generation. The current approach is predicated on the  
77 WBW model [31]—originally developed for 1 atm—, where each spectral interval's  
78 contribution is solved using the standard WBW model after the spectrum is  
79 segmented into a series of intervals. It is worth highlighting that the WBW  
80 approach is distinguished from the standard WSGG model in the sense that  
81 rather than dealing with the entire radiation spectrum at once, every spectral  
82 interval that the spectrum was split up into is individually solved and then, to  
83 get the overall result, summed the contributions of each segment. The objective  
84 here is to present a methodology which is fast and accurate with a respectable  
85 offering between computational cost and accuracy. Expressed by the radiative  
86 heat flux and radiative heat source, the accuracy results found through the  
87 present method are tested against the solutions obtained via WSGG parameters  
88 of Ref. [3] and LBL benchmark integration.

## 89 2. Radiation modeling

### 90 2.1. LBL integration method

91 The solution of thermal radiation in participating media is based on solving  
92 the RTE along a given trajectory, which it can be expressed as [1, 13]:

$$93 \quad \frac{dI_\eta}{ds} = -\kappa_\eta I_\eta + \kappa_\eta I_{b\eta}, \quad (1)$$

94 in which  $\kappa_\eta$  indicates the spectral absorption coefficient of the gas (or of a  
95 gaseous mixture),  $I_\eta$  represents the spectral radiation intensity and  $I_{b\eta}$  is the  
96 spectral blackbody radiation intensity at the temperature of the medium at the  
97 position  $s$ . On the right-hand side of the RTE, the first term corresponds to  
98 the reduction in the radiation intensity due to absorption, and the second one  
99 expresses the mechanism of emission. In Eq. (1), the scattering of radiation is  
100 neglected, which is fully justified in media formed by participating species.

101 In the present study, non-uniform temperature and concentration distribu-  
102 tions describe the participating medium formed by a H<sub>2</sub>O-CO<sub>2</sub> mixture. The  
103 absorption coefficient is obtained according to the relation below

$$104 \quad \kappa_\eta = NYC_\eta. \quad (2)$$

105 In the above equation,  $C_\eta$  is the absorption cross-section,  $Y$  is the mole fraction of  
106 the participating species and  $N$  is the molar density of the gas. The construction  
107 of the absorption spectra of the combustion byproducts, considering the collision  
108 broadening, is based on the Lorentz profile [1, 13]

$$109 \quad C_\eta = \sum_{m=1}^M \frac{S_m}{\pi} \frac{\gamma_m}{\gamma_m^2 + (\eta - \eta_m)^2}, \quad (3)$$

110 in which  $S_m$  is the  $m$ -th line integrated intensity,  $\gamma_m$  is the line half-width,  $\eta_m$   
111 is the line location and  $M$  is the amount of lines that make up the spectrum.  
112 The parameter  $\gamma_m$  is calculated accounting for the pressure and temperature  
113 according to [10]

$$114 \quad \gamma_m = \left(\frac{T_{\text{ref}}}{T}\right)^n p_e \gamma_{\text{self},m} + (p - p_e) \gamma_{\text{air},m}, \quad (4)$$

115 where  $p_e$  is the partial pressure of the participating species  $e$ ,  $\gamma_{\text{self}}$  and  $\gamma_{\text{air}}$  are  
 116 the half-widths considering the collision of gas molecules with each other and  
 117 with air molecules, respectively, and  $n$  is the temperature-dependent coefficient.  
 118 The values of  $S$ ,  $\gamma_{\text{air}}$ ,  $\gamma_{\text{self}}$  and  $n$  are obtained from a molecular spectroscopic  
 119 database.

120 In solving the energy equation, the thermal radiation can be incorporated  
 121 as a volumetric source term, directly related to the radiative flux divergence.  
 122 Solving for the spectral radiation intensity using Eq. (1), the radiative heat flux  
 123 ( $q_r$ ) divergence at each position of the medium can be determined using the  
 124 expression below:

$$125 \quad \nabla \cdot \vec{q}_r = \int_{\eta=0}^{\infty} \int_{\omega_l=0}^{4\pi} [-\kappa_{\eta} I_{\eta} + \kappa_{\eta} I_{b\eta}] d\omega_l d\eta . \quad (5)$$

126 For the radiative heat flux divergence to be determined, it needs two forms of  
 127 integration. The first one corresponds to the spatial integration, which involves  
 128 both the integration of Eq. (1) in a given direction, and the integration of  
 129 Eq. (5) in all directions in the solid angle  $d\omega_l$ . There are several spatial numeri-  
 130 cal methods, including P-N approximations, discrete ordinates method, zonal  
 131 method, Monte Carlo etc. Despite the complexity of the problem, the spatial  
 132 integration methods are well-established and can be found in specialized texts  
 133 on thermal radiation [1, 13]. The second integration corresponds to the spectral  
 134 integration of Eq. (3), which corresponds to the sum of the radiative energy  
 135 at each wavenumber  $\eta$ . The gas absorption coefficients present a very complex  
 136 behavior in relation to the wavenumber, and may be made up of millions of  
 137 absorption lines. However, the greatest difficulty lies in how the thermodynamic  
 138 state influences  $\kappa_{\eta}$ , which is even more critical in combustion processes.

## 139 2.2. WSGG model

140 The WSGG model considers that the absorption spectrum of a gas can be  
 141 divided into a gray gases set and transparent windows. In this spectral model,  
 142 the distribution of  $\kappa_{\eta}$  is normalized by the partial pressure  $p_a$  of the participating  
 143 gases,  $\kappa_{p\eta} = \kappa_{\eta}/p_a$ , for the gray gases 1 to  $J$ , distributed non-contiguously

144 along the wavenumber, with no overlap between them. Under this assumption,  
 145 the total emittance of the medium for a path-length  $L$  can be written as

$$146 \quad \varepsilon = \sum_{j=1}^J a_j(T) [1 - \exp(-\kappa_{p,j} p_a L)] , \quad (6)$$

147 where the total of the chemical species' partial pressures that form the gaseous  
 148 mixture is denoted by  $p_a$ ,  $a_j(T)$  represents the portion of blackbody energy  
 149 emanating from the spectrum's sections in which  $\kappa_{p\eta} = \kappa_{p,j}$ ; in the above  
 150 equation,  $\kappa_{p\eta} = \kappa_{\eta}/p_a$  represents the pressure-dependent spectral absorption  
 151 coefficient. In practice, the above equation corresponds to an interpolation func-  
 152 tion of total emittance data of the medium, where generally, but not necessarily,  
 153 the coefficients  $\kappa_{p,j}$  are considered constant and  $a_j$  is represented by polynomial  
 154 functions of the temperature. The determination of the total  $\varepsilon$  depends on the  
 155 integration of the spectral emittance, such that

$$156 \quad \varepsilon = \frac{\int_0^{\infty} \varepsilon_{\eta} I_{b\eta} [1 - \exp(-\kappa_{p\eta} p_a L)] d\eta}{\int_0^{\infty} I_{b\eta} d\eta} . \quad (7)$$

157 The integration of the RTE leads to

$$158 \quad \frac{dI_j}{ds} = -\kappa_{p,j} p_a I_j + \kappa_{p,j} p_a a_j I_b , \quad (8)$$

159 in which  $I_b$  represents the total blackbody radiation intensity. The overall  
 160 intensity can be determined by summing the individual intensities obtained for  
 161 each one of the gray gases,

$$162 \quad I = \sum_{j=0}^J I_j . \quad (9)$$

163 Despite its simplifications regarding the real spectrum of the gases, the WSGG model  
 164 proved capable of generating results with very satisfactory accuracy in a set of  
 165 problems with elevated temperature and concentration gradients of the involved  
 166 species, similar to those found in combustion processes [4, 6, 18, 19, 46].

### 167 2.3. WBW model

168 In spite of its simplicity by representing the spectrum commonly with only  
 169 four gray gases ( $J = 4$ ), the WSGG model is capable of obtaining solutions with



170 very satisfactory accuracy in relation to the application of the LBL integration  
 171 method, typically with maximum local errors below 10 % and average deviations  
 172 below 5 %. The computational time of the WSGG model is much lower than that  
 173 needed by the LBL benchmark solution, in the order of 0.001 %. The SLW and  
 174 FSK global models typically have greater accuracy than the WSGG model, but  
 175 they are more complex and require around five times more computational time.  
 176 Considering the long time needed to solve the RTE in problems in which the  
 177 thermal radiation is just one of the phenomena involved, such as in combustion  
 178 problems, the WSGG model may be a good option when the uncertainties  
 179 introduced by other phenomena are greater than those of the model itself.  
 180 Because of this, the present study proposes a new methodology for the WSGG  
 181 model, which consists of applying the WBW model [31] for total pressures above  
 182 the atmospheric (i.e., above 1 atm). By segmenting the spectrum into a series of  
 183  $M$  bands of width  $\Delta\eta_m$ , the proposed method seeks to widen the the standard  
 184 WSGG model accuracy using its assumptions by calculating the contributions of  
 185 all bands individually. The number  $J_m$  of gases in each band does not necessarily  
 186 need to be the same, this being an aspect that allows optimization, i.e., using a  
 187 greater or lesser number of gray gases in a interval according to their importance  
 188 in the global calculation. The results of each band are added together to calculate  
 189 the total quantities.

190 The emittance of the  $m$ -th band can be calculated by use the LBL method  
 191 of the spectral data extracted from HITEMP 2010 according to the following  
 192 equation

$$\varepsilon_m = \frac{\int_{\Delta\eta_m} I_{b\eta} [1 - \exp(-\kappa_{p\eta} p_a L)] d\eta}{\int_{\Delta\eta_m} I_{b\eta} d\eta}, \quad (10)$$

194 where  $\int_{\Delta\eta_m} I_{b\eta} d\eta = f_m I_b$ , in which  $f_m$  is the blackbody energy fraction that  
 195 emanates from each spectral band  $\Delta\eta_m$  and is calculated using the distribution  
 196 of Planck [1, 13]. With the aforementioned definition, the emittance of a band  
 197  $\varepsilon_m$  can reach a maximum value of 1, as well as the total emittance defined in  
 198 Eq. (7), which are related as  $\varepsilon = \sum_{m=1}^M f_m \varepsilon_m$ .

199 With the other WBW assumptions being equivalent to those of the WSGG

200 model, for each band the value of  $\varepsilon$  as follow as

$$201 \quad \varepsilon_m = \sum_{j=1}^{J_m} a_{j,m}(T) [1 - \exp(-\kappa_{p,j,m} p_a L)] , \quad (11)$$

202 in which  $a_{j,m}$  is the temperature-dependent coefficient,  $\kappa_{p,j,m}$  is the pressure-  
 203 dependent coefficient—both related to the gray gas  $j$  and band  $m$ . Finally, as  
 204 in the classic model, the coefficients of the WBW model are determined by  
 205 correlating Eq. (11) with the values of emittance of the bands calculated via  
 206 LBL integration of Eq. (10), considering the coefficients  $\kappa_{p,j,m}$  as constant and  
 207 the coefficients  $a_{j,m}$  are represented by temperature polynomial functions.

208 The RTE, in the context of the proposed method, is given by

$$209 \quad \frac{dI_{j,m}}{ds} = -\kappa_{p,j,m} p_a I_{j,m} + \kappa_{p,j,m} p_a a_{j,m} f_m I_b , \quad (12)$$

210 where the blackbody energy emission in the wide-band  $m$  is weighted by  $f_m$ , the  
 211 overall radiation intensity is computed as the total of the individual intensities  
 212 calculated for each gray gas  $j$ , according to the equation below

$$213 \quad I = \sum_{m=1}^M \sum_{j=0}^J I_{j,m} , \quad (13)$$

214 and  $a_{j,m}$  is fitted using a temperature polynomial function

$$215 \quad a_{j,m}(T) = \sum_{k=0}^{\mathcal{K}} b_{j,m,k} T^k , \quad (14)$$

216 with  $b_{j,m,k}$  displaying the coefficients of the temperature polynomial of the order  $k$   
 217 for the gray gas  $j$  and band  $m$ . In a participating medium enclosed by boundaries  
 218 that are black, Eq. (12) is constrained by the boundary condition:  $I_{j,m}|_{\text{wall}} =$   
 219  $(a_{j,m} f_m I_b)|_{\text{wall}} = a_{j,m}(T_w) f_m(T_w) I_b(T_w)$ . The terms of the boundary condition  
 220 are all evaluated in relation to the wall temperature  $T_w$ , which, in the present  
 221 paper, is prescribed for all test cases investigated here.

222 Finally, by integrating the RTE and resolving the intensities for  $n_d$  directions,

223  $q_r$  and radiative heat source,  $S_r$ , at each point can be computed as

$$224 \quad q_r(x) = \sum_{m=1}^M \sum_{l=1}^{n_d} \sum_{j=0}^J 2\pi\mu_l\omega_l \left[ I_{j,l,m}^+(x) - I_{j,l,m}^-(x) \right], \quad (15)$$

$$225 \quad S_r(x) = \sum_{m=1}^M \sum_{l=1}^{n_d} \sum_{j=1}^J 2\pi\kappa_{pj,m}p_a\omega_l \left[ I_{j,l,m}^+(x) + I_{j,l,m}^-(x) \right] - 4\pi\kappa_{pj,m}p_a a_{j,m} f_m I_b(x),$$

226 (16)

227 in which  $I_{j,l,k}^-$  and  $I_{j,l,k}^+$  are the gray gas radiation intensities in the negative and  
 228 positive directions, respectively,  $\omega_l$  are the weights of the quadrature and  $\mu_l$  are  
 229 the direction cosines. The full WBW model formulation is available in [31] for a  
 230 more thorough understanding.

### 231 3. Results and discussions

232 In the present paper, the formulation is implemented to a 1D system, in  
 233 which the plates are black and separated by  $X = 1$  m, illustrated in Fig. 1. The  
 234 fixed mole fraction of the medium is  $p_w/p_c = 2$  and it experiences three total  
 235 pressures: 1 atm, 10 atm and 20 atm. Using the direction cosines and weights  
 236 presented in Ref. [47], the RTE directional integration was completed via discrete  
 237 ordinates method for 8 directions; 200 equally spaced cells were used for the  
 238 discretization of the computational domain spatial mesh. These parameters were  
 239 chosen through complementary studies analyzing the quality of the spatial and  
 240 directional meshes, which demonstrated that a higher level of refinement had  
 241 no impact on the accuracy of the solutions, so that the values adopted for the  
 242 problem under study were considered adequate. As shown in Table 1, five spectral  
 243 bands was the quantity of divisions into which the spectrum was fractioned. The  
 244 criteria to establish the division of the bounds of each band are the same used  
 245 by Refs. [31, 48]. Fixed mole fractions of  $Y_c = 0.1$  and  $Y_w = 0.2$  (with the  
 246 letters  $c$  and  $w$  standing for carbon dioxide and water vapor, respectively), and  
 247 43 values of  $L$  (ranging from 0.001 m up to 30 m) were adopted to generate the  
 248 band emittances. Although the WBW model, in its your original formulation,  
 249 has already provided correlations for the case in which the total pressure is 1 atm

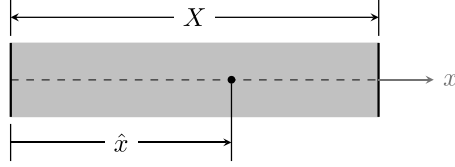


Figure 1: Schematic of the computational domain.

Table 1: Bounds of the spectral bands evaluated in this paper.

Spectral band	$\eta_l$ [ $\text{cm}^{-1}$ ]	$\eta_u$ [ $\text{cm}^{-1}$ ]
1	0	1000
2	1000	2600
3	2600	4400
4	4400	6000
5	6000	10000

250 through Ref. [31], new coefficients were produced for this value of  $p$ , since the  
 251 upper limit of the final interval in that paper was different from the case under  
 252 study here. Due to the similarity between the coefficients proposed by [31], even  
 253 though the last spectral band is slightly different, it was decided to omit the  
 254 WBW coefficients for 1 atm. For the other values of total pressure under study  
 255 here, the WBW correlations are available in Appendix A.

256 The temperature and medium composition profiles are described by a set of  
 257 cases. Case 1 presents simple symmetry regarding the  $x$ -axis, and its behaviors  
 258 for the temperature profile and mole fraction of carbon dioxide are expressed,  
 259 respectively, as

$$260 \quad T(\hat{x}) = 400 + 1400 \sin^2(\pi \hat{x}), \quad (17)$$

$$261 \quad Y_c(\hat{x}) = 0.1 \sin^2(\pi \hat{x}), \quad (18)$$

262 where the parameter  $\hat{x}$  represents the dimensionless distance relative to the left  
 263 boundary ( $\hat{x} = x/X$ ). In the second case,  $T$  and  $Y_c$  present double symmetry,  
 264

265 and these two quantities are described, respectively, by

$$266 \quad T(\hat{x}) = 400 + 1400 \sin^2(2\pi\hat{x}), \quad (19)$$

$$267 \quad Y_c(\hat{x}) = 0.1 \sin^2(2\pi\hat{x}). \quad (20)$$

269 The profiles described in Eqs. (17) and (19) have a maximum value of temperature  
 270 at 1800 K and an average temperature of 1100 K. In Eqs. (18) and (20) the peak  
 271 of carbon dioxide mole fraction is 0.1 and the value average of the medium  
 272 composition is 0.05. Another set of temperature is also tested, but with the  
 273 average and maximum temperatures of 1300 K and 2200 K, respectively, as  
 274 follows

$$275 \quad T(\hat{x}) = 400 + 1800 \sin^2(2\pi\hat{x}), \quad (21)$$

$$276 \quad T(\hat{x}) = \begin{cases} 880 + 1320 \sin^2(2\pi\hat{x}), & \text{if } \hat{x} \leq 0.25, \\ 400 + 1800 \left\{ 1 - \sin^{\frac{3}{2}} \left[ \frac{2\pi}{3} (\hat{x} - 0.25) \right] \right\}, & \text{if } \hat{x} > 0.25. \end{cases} \quad (22)$$

278 Regarding the above profiles, Case 3 combines Eqs. (18) and (21) for CO<sub>2</sub> mole  
 279 fraction and temperature profiles, respectively. Finally, Case 4 is represented by  
 280 Eqs. (20) and (22) for the carbon dioxide mole fraction and temperature profiles,  
 281 respectively. In Cases 1 to 3, both walls are at a temperature of 400 K. In Case 4,  
 282 the left boundary is at 880 K while the right wall is at 400 K.

283 With the objective of optimizing the computational cost required to generate  
 284 the results for the WBW model, the quantity of gray gases spread within each  
 285 segment in the four test cases under investigation in this paper was varied  
 286 between the values of two and four. It was decided to adopt this quantity of  
 287 gray gases in each spectral interval based on the study carried out by [31], in  
 288 which it was found that it is appropriate to distribute a greater number of  
 289 gases to the most important bands and a smaller number to the less important  
 290 ones. In Approach A, a total of 20 gray gases are distributed across the five  
 291 bands. In Approach B, 14 gases are used to represent the proposed method.  
 292 And, in Approaches C and D, are distributed a total of 12 and 16 gray gases,  
 293 respectively, along the spectrum. Further, the results obtained by Approaches

Table 2: Gray gases quantity in each interval for each one of the tested WBW approaches.

Approach	Band 1	Band 2	Band 3	Band 4	Band 5	Total
A	4	4	4	4	4	20
B	2	4	4	2	2	14
C	2	3	3	2	2	12
D	2	3	3	4	4	16

294 A–D are obtained through combinations of the sets of correlations presented in  
 295 Appendix A. Table 2 presents a summary with the number of gray associated to  
 296 each band for each approach.

297 To measure the accuracy of the proposed formulation regarding the LBL  
 298 method, maximum and average normalized deviations were calculated, according  
 299 to the equation below:

$$300 \quad \delta\phi = \frac{|\phi_{\text{LBL}} - \phi_{\text{app}}|}{\max(|\phi_{\text{LBL}}|)} \times 100\%. \quad (23)$$

301 In the above equation,  $\phi$  is either  $q_r$  and  $S_r$ , the subscript “app” indicates the  
 302 tested approach against the LBL method (indicated by the subscript “LBL”),  
 303 and  $\max(|\phi_{\text{LBL}}|)$  represents the maximum absolute value for  $q_r$  or  $S_r$  obtained  
 304 by the reference solution. Later, the maximum and average deviations in relation  
 305 to the benchmark solution will be indicated by the use of the subscripts “max”  
 306 and “avg”, respectively.

307 Using the methodology outlined in Ref. [3], the absorption spectra of  $\text{CO}_2$   
 308 and  $\text{H}_2\text{O}$  at high pressures were generated from the HITEMP 2010. All five  
 309 of the intervals’ emittances were obtained via Eq. (10), and the adjustments  
 310 of  $\varepsilon$  were completed in an analogous way to that reported in Ref. [31]. The  
 311 function presented in Eq. (11) was employed in order to fit the proposed model’s  
 312 parameters. As in Ref. [31], the WBW correlations were generated assuming a  
 313 number between two and four to describe the amount of gray gases in each band,  
 314 adopting a polynomial of fifth order to describe the dependence on temperature.  
 315 The emittance charts for 10 atm and 20 atm are shown in Figs. 2 and 3. The  $\varepsilon$

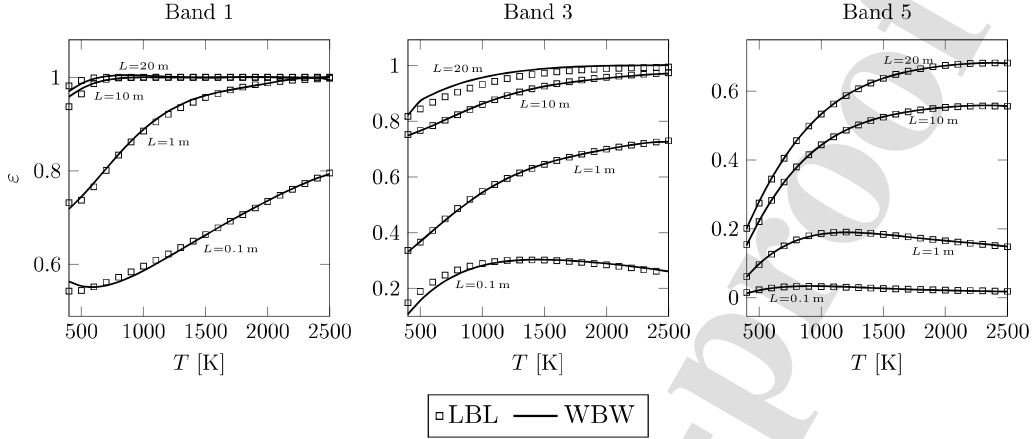


Figure 2: Emittances of three of the selected bands and  $p = 10$  atm.

316 values depicted in these figures illustrate the solutions found with the WBW  
 317 model considering four gray gases per interval. Only 4 of the values of  $L$  that  
 318 were used to calculate  $\varepsilon$  were displayed in the figures for the sake of brevity; the  
 319 remaining path-lengths exhibit tendencies that are similar to what is addressed  
 320 next.

321 At a total pressure of  $p = 10$  atm, the results illustrated in Fig. 2 demonstrate  
 322 a good fit between the WBW model and the LBL integration method, with a  
 323 maximum relative error (determined as  $|\varepsilon_{\text{LBL}} - \varepsilon_{\text{WBW}}|/\varepsilon_{\text{LBL}} \times 100\%$ ) of less  
 324 than 2%, occurring in the areas with cooler temperatures. Given that the WBW  
 325 model outperformed the benchmark solution, the polynomial fitting is deemed  
 326 adequate for the purposes of this paper's analysis.

327 The emittances for the three bands produced using the WBW model and the  
 328 LBL method for  $p = 20$  atm are compared in Fig. 3. At contrast to  $p = 10$  atm,  
 329 2.1% was the maximum local deviation found at the temperature-highest region,  
 330 where the biggest disparity between the two methods was observed. Despite  
 331 the omission of  $\varepsilon$  results for 1 atm, the deviations for the other values of total  
 332 pressure are comparable to those that were disclosed by [31], corroborating the  
 333 suitability of the polynomial fitting.

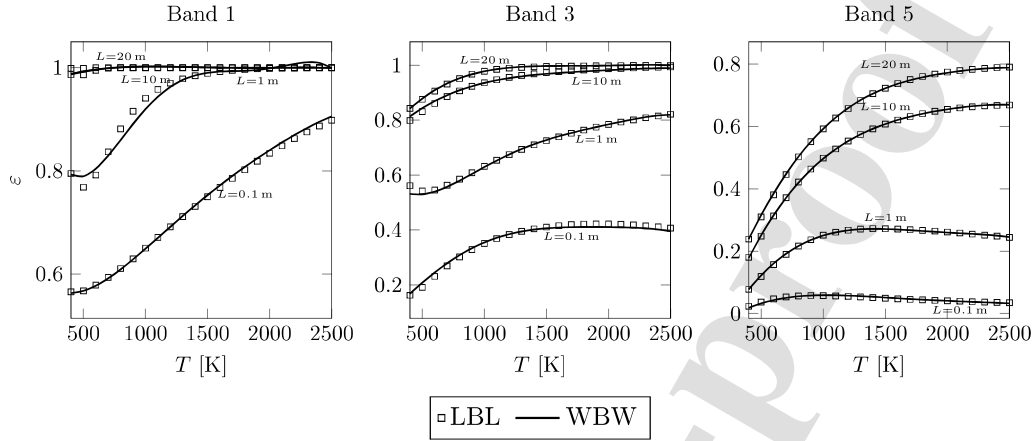


Figure 3: Emittances of three of the selected bands and  $p = 20$  atm.

334 The WBW model is now used to calculate  $q_r$  and  $S_r$  for the four case  
 335 studies that were described. The pressures of 1 atm to 20 atm are displayed  
 336 in the following figures together with  $q_r$  and  $S_r$  for each case. Calculations  
 337 for atmospheric pressure were carried out with the WBW model coefficients  
 338 presented in [31], but with new correlations generated for the last spectral  
 339 band. The results obtained by applying the WBW model, assuming that there  
 340 are two to four gray gases in each spectral band, are plotted in Figs. 4–7.  
 341 Additionally, under the identical physical conditions, these diagrams show the  
 342 resulting curves produces by applying the WSGG coefficients that were generated  
 343 by [3]. The goal is to assess whether the proposed methodology’s accuracy might  
 344 be improved upon in comparison to an alternative WSGG model formulation  
 345 for high pressures that is currently existing in the literature. Tables 3 and 4  
 346 provide a summary of the average and maximum normalized errors with the  
 347 LBL method in comparison to the WSGG and WBW models, respectively. In  
 348 order not to impair the understanding of the figures with the results, only the  
 349 curves that describe the solutions containing four gray gases in each band were  
 350 plotted in Figs. 4–7 (curves “WBW-A” in these figures). The performance of the  
 351 other solutions (Approaches B to D) are expressed only in terms of maximum



352 and average errors regarding the reference solution and can be seen in Table 4.

353 Figure 4 presents  $q_r$  and  $S_r$  results for Case 1 for the WBW and WSGG  
 354 approaches against the LBL integration for the three total pressures assessed  
 355 in this paper. When comparing the two methods studied in this paper with  
 356 respect to the LBL solution, a good agreement is found between the WBW  
 357 model and the LBL method throughout the three total pressure values for  $q_r$   
 358 and  $S_r$ . Although the atmospheric pressure does not characterize a high pressure  
 359 scenario, it was decided to also present the results obtained with 1 atm, so that  
 360 the performance of the proposed method could be evaluated as the value of  
 361 the total pressure system rises. Thus, for 1 atm, Table 3 shows that the biggest  
 362 errors obtained via WSGG model of Ref. [3] for 1 atm are 5.1 % and 3.2 %,   
 363 respectively. According to Table 4, all the four approaches of the WBW model  
 364 presented a better performance for the atmospheric pressure in comparison with  
 365 the WSGG model. The results with greater accuracy were obtained with the  
 366 Approach A of the WBW model, with maximum errors of 3.0 % for  $q_r$  and 3.4 %  
 367 for  $S_r$ . With Approach C, which presents 12 gray gases distributed throughout  
 368 the spectrum, the WBW model also presented smaller deviations compared  
 369 to the WSGG model, with maximum errors of 4.1 % ( $q_r$ ) and 3.1 % ( $S_r$ ). For  
 370  $p = 10$  atm, the WSGG model provides maximum errors of 5.6 % and 3.8 %  
 371 for  $q_r$  and  $S_r$ , respectively. With the WBW model, the Approaches B and D  
 372 carried out to the best results, such that: for  $q_r$ , the maximum errors were  
 373 1.8 % (Approach B) and 1.3 % (Approach D); for  $S_r$ , the maximum deviations  
 374 were 0.7 % (Approach B) and 0.6 % (Approach D). For 20 atm, the maximum  
 375 deviations with the WSGG model were 3.4 %, for  $q_r$ , and 3.8 %, for  $S_r$ . Again,  
 376 all the tested WBW approaches presented a superior accuracy compared to the  
 377 WSGG model, with the Approaches A and C reaching the most accurate results:  
 378 1.4 % and 1.35 % for the radiative heat flux, respectively, and 0.6 % and 0.7 % for  
 379 the radiative heat source, respectively. These results show that highlight the fact  
 380 that optimizing the gray gases number distributed in each interval can further  
 381 improve the results, which were already better than those obtained through the  
 382 WSGG correlations proposed by Ref. [3].

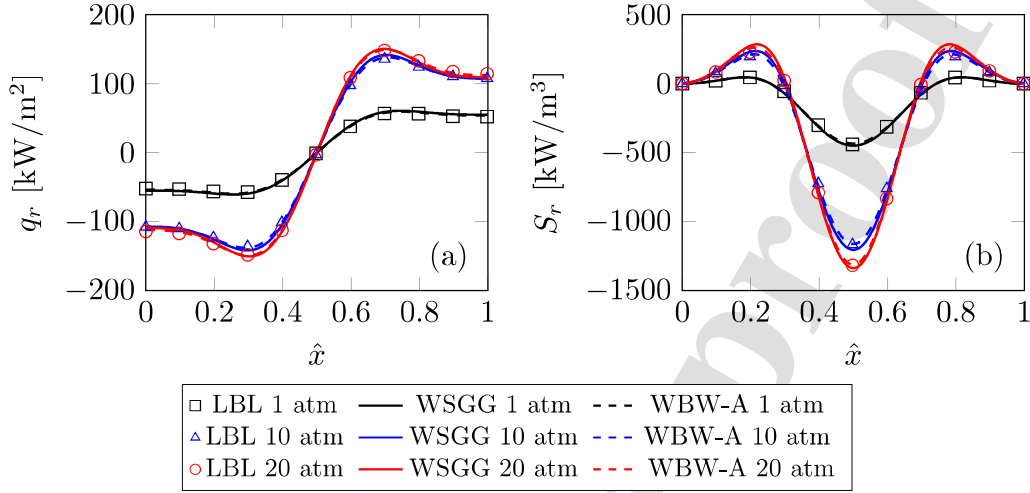


Figure 4: Case 1: (a) radiative heat flux; (b) radiative heat source.

Table 3: Percentage deviations of  $q_r$  and  $S_r$  between the WSGG model of Ref. [3] and the reference solution.

	$p = 1 \text{ atm} [\%]$				$p = 10 \text{ atm} [\%]$				$p = 20 \text{ atm} [\%]$			
	$(\delta q_r)_{\max}$	$(\delta q_r)_{\text{avg}}$	$(\delta S_r)_{\max}$	$(\delta S_r)_{\text{avg}}$	$(\delta q_r)_{\max}$	$(\delta q_r)_{\text{avg}}$	$(\delta S_r)_{\max}$	$(\delta S_r)_{\text{avg}}$	$(\delta q_r)_{\max}$	$(\delta q_r)_{\text{avg}}$	$(\delta S_r)_{\max}$	$(\delta S_r)_{\text{avg}}$
Case 1	5.10	3.67	3.22	1.38	5.61	2.39	3.80	2.14	3.37	1.83	3.82	1.61
Case 2	5.24	2.50	6.21	1.97	5.51	3.32	8.08	2.71	7.09	3.10	7.95	2.96
Case 3	7.20	3.47	7.54	2.47	5.27	2.13	3.74	1.61	5.48	3.22	6.44	2.33
Case 4	10.36	5.41	7.42	1.74	4.13	1.75	4.73	1.01	5.22	2.28	5.48	1.22

383 For Case 2, Fig. 5 displays  $q_r$  and  $S_r$  for each one of the three total pressure  
 384 values. Once again, there was a good match between the LBL and WBW  
 385 solutions, with the latter performing superior to the WSGG model, since, the  
 386 Case 1, the proposed method showed the least inaccuracy with respect to the  
 387 LBL integration. Based on Tables 3 and 4, for 1 atm, the maximum deviations  
 388 were obtained with the Approaches A and B, being 3.6% and 4.1%, respectively,  
 389 for  $q_r$ , and 4.0% and 3.7%, respectively, for  $S_r$ , against 5.2% ( $q_r$ ) and 6.2%  
 390 ( $S_r$ ) via WSGG approach. For 10 atm, the Approaches C and D presented the  
 391 best performances, with maximum deviations of 2.6% and 2.0%, respectively,

Table 4: Percentage deviations of  $q_r$  and  $S_r$  between the proposed method and the reference solution.

	$(\delta q_r)_{\max}$	$(\delta q_r)_{\text{avg}}$	$(\delta S_r)_{\max}$	$(\delta S_r)_{\text{avg}}$	$(\delta q_r)_{\max}$	$(\delta q_r)_{\text{avg}}$	$(\delta S_r)_{\max}$	$(\delta S_r)_{\text{avg}}$
	WBW Approach A [%]				WBW Approach B [%]			
$p = 1 \text{ atm}$								
Case 1	3.03	1.87	3.36	1.09	3.59	2.30	3.17	1.01
Case 2	3.60	1.50	4.04	1.54	4.09	1.76	3.73	1.38
Case 3	4.06	1.77	6.02	2.46	4.70	2.10	5.05	2.19
Case 4	4.16	2.57	6.25	1.45	4.72	2.21	5.99	1.36
$p = 10 \text{ atm}$								
Case 1	2.01	0.89	1.78	0.68	2.11	1.24	1.26	0.59
Case 2	2.81	1.17	2.47	0.95	2.89	1.22	2.41	0.90
Case 3	5.28	2.13	3.67	1.55	6.90	2.99	2.88	1.38
Case 4	4.35	2.34	4.67	1.34	6.61	3.61	4.38	0.64
$p = 20 \text{ atm}$								
Case 1	1.37	0.63	2.11	0.70	1.35	0.73	2.14	0.66
Case 2	2.41	0.78	4.66	1.39	1.85	1.04	4.43	1.24
Case 3	2.88	1.18	4.16	1.47	2.48	0.84	3.67	1.23
Case 4	3.23	1.24	4.44	0.81	4.86	1.08	5.04	1.34
	WBW Approach C [%]				WBW Approach D [%]			
$p = 1 \text{ atm}$								
Case 1	4.13	2.95	3.09	1.17	3.96	2.78	3.05	1.13
Case 2	5.42	2.42	4.31	1.84	5.26	2.33	4.06	1.80
Case 3	4.93	1.87	4.01	1.42	4.53	1.65	3.95	1.33
Case 4	6.65	4.68	4.70	1.11	8.73	4.29	4.60	1.11
$p = 10 \text{ atm}$								
Case 1	1.53	0.90	1.62	0.49	1.60	0.67	2.23	0.82
Case 2	2.62	0.99	1.99	0.85	2.04	0.73	2.22	1.03
Case 3	5.15	2.19	3.76	1.11	3.07	1.17	2.27	0.86
Case 4	4.20	2.24	4.38	0.80	1.92	0.86	3.35	0.70
$p = 20 \text{ atm}$								
Case 1	0.82	0.39	1.23	0.48	2.35	1.56	3.06	0.99
Case 2	1.92	0.90	2.86	0.84	2.50	0.58	3.42	1.03
Case 3	3.50	1.62	2.05	0.94	1.84	0.75	3.31	1.32
Case 4	2.93	1.10	2.36	0.60	2.85	0.76	3.45	0.90

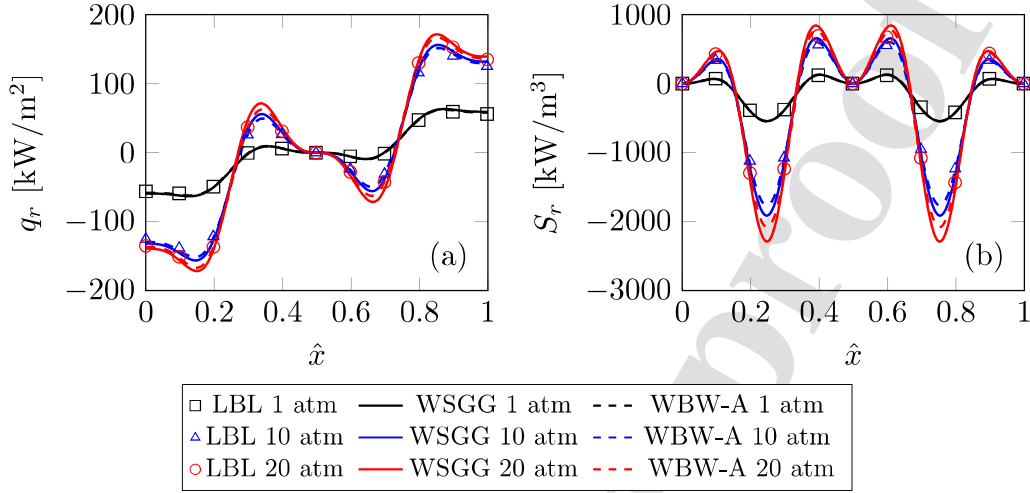


Figure 5: Case 2: (a) radiative heat flux; (b) radiative heat source.

392 for  $q_r$ , and 2.0% and 2.2%, respectively, for  $S_r$ . The WSGG model, in turn,  
 393 reached maximum deviations of 5.5%, for  $q_r$ , and 8.1%, for  $S_r$ . For the third  
 394 value of total pressure tested in this paper (i.e., 20 atm), the Approaches B  
 395 and C carried out to the smallest errors, whose magnitudes of deviations for  
 396  $q_r$  and  $S_r$  were 1.8% and 4.4%, respectively, with the first one, and 1.9% and  
 397 2.9%, respectively, with the second one. Meanwhile, the WSGG model, in turn,  
 398 provided maximum errors of 7.1% and 7.9% for the radiative heat flux and  
 399 radiative heat source, respectively. Again, the WBW solution demonstrated to  
 400 be a superior substitute for calculating the radiative transfer compared to the  
 401 standard WSGG model, since the results obtained with the proposed method  
 402 presented more accuracy.

403 The results depicted in Fig. 6 show  $q_r$  and  $S_r$  for Case 3 for the three values  
 404 of pressure under consideration. According to data from Table 3, for the three  
 405 values of total pressure, the worst results were obtained for 1 atm, with maximum  
 406 errors of 7.2%, for  $q_r$ , and 7.5%, for  $S_r$ . These deviations decrease with the  
 407 increase of the total pressure, becoming 5.3% and 3.7%, for  $p = 10$  atm, and 5.5%  
 408 and 6.4%, for  $p = 20$  atm. Regarding the WBW model, all the tested approaches

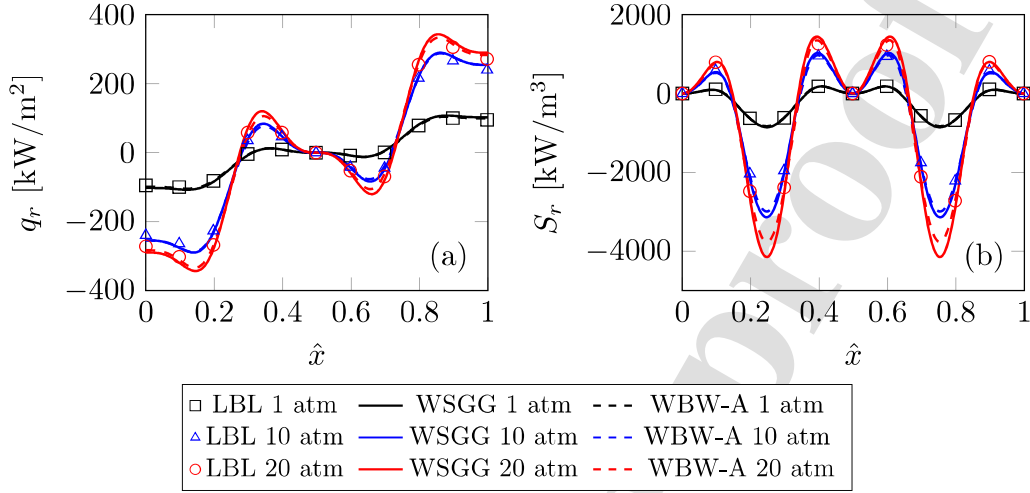


Figure 6: Case 3: (a) radiative heat flux; (b) radiative heat source.

409 performed better compared to the classic version of the WSGG model, since the  
 410 discrepancies regarding the LBL solution were less than those calculated by the  
 411 WSGG coefficients proposed by Ref. [3]. For 1 atm, the best performances of  
 412 the WBW model were obtained with the Approaches C and D, with maximum  
 413 deviations of 4.9% and 4.5%, respectively, for the radiative heat flux, and  
 414 4.0% and 3.9%, respectively, for the radiative heat source. For  $p = 10$  atm,  
 415 Approaches C and D presented the smallest deviations for the radiative heat  
 416 flux, with magnitudes of 5.1% and 3.1%, respectively; for the radiative heat  
 417 source, Approaches B and D reached the best results, with maximum deviations  
 418 of 2.9% and 2.8%, respectively. For  $p = 20$  atm, again Approaches C and D  
 419 presented the best performances, being 3.5% and 1.8% the maximum errors  
 420 obtained for  $q_r$ , and 2.0% and 3.3% the deviations for  $S_r$ , respectively.

421 Finally, Fig. 7 shows the results for  $q_r$  and  $S_r$  for Case 4 for all the analyzed  
 422 values of total pressure. As in previous test cases, the proposed method outper-  
 423 formed the standard WSGG model. For the first value of total pressure evaluated  
 424 (i.e.,  $p = 1$  atm), the maximum error for the radiative heat flux exceeded 10%;  
 425 for the radiative heat source, the performance of the WSGG model was not very

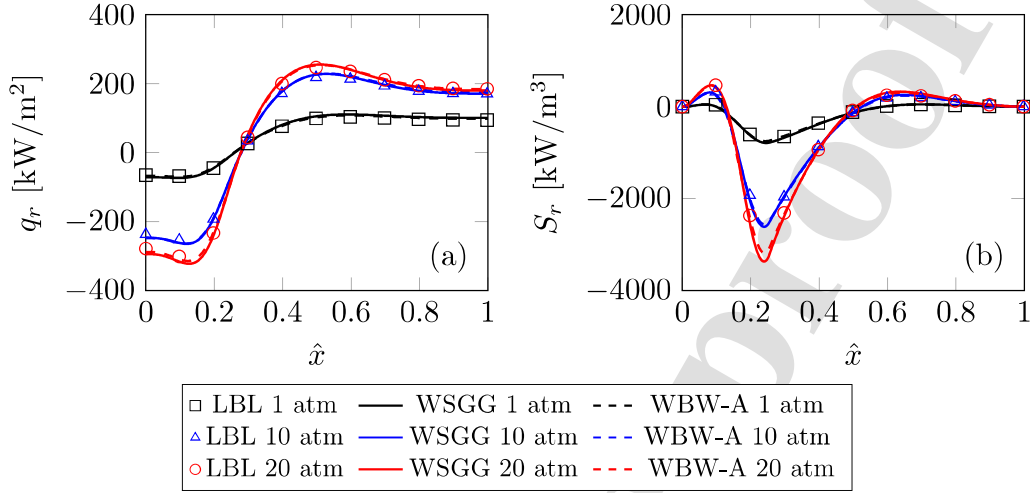


Figure 7: Case 4: (a) radiative heat flux; (b) radiative heat source.

426 good either, with 7.4 % of deviation. The results for the highest pressures, 10 atm  
 427 and 20 atm, were slightly better, with maximum deviations whose magnitudes  
 428 were 4.1 % and 5.2 %, respectively, for  $q_r$ , and 4.7 % and 5.5 %, respectively, for  
 429  $S_r$ . Analogously to what was observed with the WSGG model, Case 4 was the  
 430 one that had the biggest errors regarding the LBL method, in contrast to the  
 431 other test cases studied. Still, on average, the WBW model presented a better  
 432 performance in comparison to the standard WSGG model. The Approaches A  
 433 and B presented the smallest deviations, being 4.2 % and 4.7 %, respectively,  
 434 for the radiative heat flux, and 6.6 % for both approaches, for the radiative  
 435 heat source, for  $p = 1$  atm. For the intermediate value of total pressure (i.e.,  
 436  $p = 10$  atm), the best performances were obtained by Approaches C and D, in  
 437 which the maximum deviations 4.2 % ( $q_r$ ) and 1.9 % ( $S_r$ ), with the first one, and  
 438 4.4 % ( $q_r$ ) and 3.3 % ( $S_r$ ), for the second one. For the last value of total pressure  
 439 (i.e., 20 atm), the smallest errors also were provided through Approaches C and  
 440 D, whose the magnitudes were 2.9 % and 2.8 %, respectively, for  $q_r$ , and 2.4 %  
 441 and 3.4 %, respectively, for  $S_r$ .

442 Additionally, it is important to highlight that the solution with 20 gray gases

443 (Approach A) is equivalent to a classic approach of the SLW model, which uses  
444 from 20 to 25 gases distributed throughout the entire spectrum. Therefore, by  
445 reducing from 20 to 12 gray gases, the WBW model will decrease the number of  
446 equations to be solved, which, in turn, reduces the computational time required  
447 to run the same test case. So, the Approach D, which in some cases led to the  
448 smallest deviations in relation to the benchmark solution, represents a significant  
449 reduction in the computational cost, since it will be necessary to solve the RTE  
450 only 12 times, i.e., once for each gray gas, instead of solving this equation 20  
451 times. Thus, it is noted that the optimized approaches of the WBW model  
452 become competitive in relation to the SLW model, since the computational time  
453 required is less, in addition to having just as good accuracy. In future studies, it  
454 is planned to numerically compare optimized approaches of the WBW model  
455 with some formulations of the SLW model.

#### 456 4. Conclusions

457 A WBW model extension for estimating the radiative transfer at high pres-  
458 sures was carried out in this paper. Based on the LBL data of the emittance for  
459 1 atm to 20 atm, correlation sets for the proposed model were developed. The  
460 proposed method involves optimizing the standard WSGG model through the  
461 division of the spectrum into a series of segments. The results obtained with  
462 the model that was firstly proposed by [31] for atmospheric pressure showed  
463 that the WBW model can be successfully employed at high pressures scenar-  
464 ios, as evidenced by the deviations for the prediction of the emittance about  
465 2%. The accuracy of the present formulation was evaluated for four cases with  
466 non-uniform temperature and concentration  $\text{CO}_2/\text{H}_2\text{O}$  mixtures. The maximum  
467 errors were of the order of 5% regarding the LBL integration for  $q_r$  and  $S_r$ .  
468 Although not very common, the worst results, whose errors exceeded 6%, were in  
469 cases where even the standard WSGG model presented even lower performance.  
470 In addition, the tested approaches showed that one of the ways to improve the  
471 proposed formulation would be to carry out more in-depth studies to weight the

472 importance of the spectral bands, in order to optimize the gray gases quantity,  
473 leading to more accurate results with less computational time. Furthermore,  
474 new correlations are being produced for variable mole fraction ratios of water  
475 vapor and carbon dioxide, in order to increase the flexibility and applicability of  
476 the proposed model to larger variety of engineering problems. Apart from this,  
477 the fact of making the formulation adaptable and suitable to other combustion  
478 situations, new WBW coefficients are also being produced for different  $\text{H}_2\text{O}-\text{CO}_2$   
479 mole fraction ratios. Comparisons with other more advanced spectral models  
480 (such as SLW, FSCCK etc.) could also be addressed in future studies. Another  
481 possibility for the continuity of the research is to apply the present WBW model  
482 in the solution of non-gray boundaries and high pressure conditions. This topic  
483 has already begun to be explored with the preliminary work of Ref. [49], in which  
484 the WBW model showed a higher accuracy than conventional box models, with  
485 maximum errors of 4%, and which will be investigated in more detail in future  
486 studies.

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#### 491 **References**

- 492 [1] M. F. Modest, Radiative Heat Transfer, Academic Press, 2013.
- 493 [2] M. F. Modest, D. C. Haworth, Radiative Heat Transfer in Turbulent Com-  
494 bustion Systems: Theory and Applications, Springer, 2016.
- 495 [3] F. R. Coelho, F. H. R. França, WSGG correlations based on HITEMP2010  
496 for gas mixtures of  $\text{H}_2\text{O}$  and  $\text{CO}_2$  in high total pressure conditions,  
497 International Journal of Heat and Mass Transfer 127 (2018) 105–114.  
498 doi:10.1016/j.ijheatmasstransfer.2018.07.075.



- 499 [4] B. Wang, Y. Xuan, An improved WSGG model for exhaust gases of aero  
500 engines within broader ranges of temperature and pressure variations,  
501 International Journal of Heat and Mass Transfer 136 (2019) 1299–1310.  
502 doi:10.1016/j.ijheatmasstransfer.2019.03.105.
- 503 [5] H. Bordbar, F. R. Coelho, G. C. Fraga, F. H. França, S. Hostikka, Pressure-  
504 dependent weighted-sum-of-gray-gases models for heterogeneous CO<sub>2</sub>-H<sub>2</sub>O  
505 mixtures at sub- and super-atmospheric pressure 173 (2021) 121207. doi:  
506 10.1016/j.ijheatmasstransfer.2021.121207.
- 507 [6] Q. Zhang, S. Shan, Z. Zhou, K. H. Luo, A new WSGG radiation model of  
508 CO/CO<sub>2</sub> mixed gas for solar-driven coal/biomass fuel gasification, Fuel 346  
509 (2023) 128241. doi:10.1016/j.fuel.2023.128241.
- 510 [7] T. F. Wall, Combustion processes for carbon capture, Proceedings of the  
511 Combustion Institute 31 (1) (2007) 31–47. doi:10.1016/j.proci.2006.  
512 08.123.
- 513 [8] T. Wall, R. Stanger, S. Santos, Demonstrations of coal-fired oxy-fuel technol-  
514 ogy for carbon capture and storage and issues with commercial deployment  
515 5 (2011) 5–15.
- 516 [9] Z. Chen, X. Qin, B. Xu, Y. Ju, F. Liu, Studies of radiation absorption  
517 on flame speed and flammability limit of CO<sub>2</sub> diluted methane flames at  
518 elevated pressures, Proceedings of the Combustion Institute 31 (2) (2007)  
519 2693–2700.
- 520 [10] L. Rothman, I. Gordon, R. Barber, H. Dothe, R. Gamache, A. Goldman,  
521 V. Perevalov, S. Tashkun, J. Tennyson, HITEMP, the high-temperature  
522 molecular spectroscopic database, Journal of Quantitative Spectroscopy  
523 and Radiative Transfer 111 (15) (2010) 2139–2150. doi:10.1016/j.jqsrt.  
524 2010.05.001.
- 525 [11] I. Gordon, L. Rothman, R. Hargreaves, R. Hashemi, E. Karlovets, F. Skinner,  
526 E. Conway, C. Hill, R. Kochanov, Y. Tan, P. Wcisło, A. Finenko, K. Nelson,

- 527 P. Bernath, M. Birk, V. Boudon, A. Campargue, K. Chance, A. Coustenis,  
528 B. Drouin, J. Flaud, R. Gamache, J. Hodges, D. Jacquemart, E. Mlawer,  
529 A. Nikitin, V. Perevalov, M. Rotger, J. Tennyson, G. Toon, H. Tran,  
530 V. Tyuterev, E. Adkins, A. Baker, A. Barbe, E. Canè, A. Császár, A. Dudary-  
531 onok, O. Egorov, A. Fleisher, H. Fleurbaey, A. Foltynowicz, T. Furtenbacher,  
532 J. Harrison, J. Hartmann, V. Horneman, X. Huang, T. Karman, J. Karns,  
533 S. Kassı, I. Kleiner, V. Kofman, F. Kwabia-Tchana, N. Lavrentieva, T. Lee,  
534 D. Long, A. Lukashetskaya, O. Lyulin, V. Makhnev, W. Matt, S. Massie,  
535 M. Melosso, S. Mikhailenko, D. Mondelain, H. Müller, O. Naumenko, A. Per-  
536 rin, O. Polyansky, E. Raddaoui, P. Raston, Z. Reed, M. Rey, C. Richard,  
537 R. Tóbiás, I. Sadiq, D. Schwenke, E. Starikova, K. Sung, F. Tamassia,  
538 S. Tashkun, J. Vander Auwera, I. Vasilenko, A. Vıgasin, G. Villanueva,  
539 B. Vispoel, G. Wagner, A. Yachmenev, S. Yurchenko, The HITRAN2020  
540 molecular spectroscopic database, *Journal of Quantitative Spectroscopy and*  
541 *Radiative Transfer* (2021) 107949doi:10.1016/j.jqsrt.2021.107949.
- 542 [12] J. Taine, A line-by-line calculation of low-resolution radiative properties of  
543 CO<sub>2</sub>-CO-transparent nonisothermal gases mixtures up to 3000 K, *Journal*  
544 *of Quantitative Spectroscopy and Radiative Transfer* 30 (4) (1983) 371–379.  
545 doi:10.1016/0022-4073(83)90036-5.
- 546 [13] J. R. Howell, M. P. Mengüç, R. Siegel, *Thermal Radiation Heat Transfer*,  
547 6th Edition, CRC press, 2016.
- 548 [14] M. F. Modest, H. Zhang, The full-spectrum correlated-*k* distribution for  
549 thermal radiation from molecular gas-particulate mixtures, *Journal of Heat*  
550 *Transfer* 124 (1) (2002) 30–38. doi:10.1115/1.1418697.
- 551 [15] M. K. Denison, B. W. Webb, A spectral line-based weighted-sum-of-gray-  
552 gases model for arbitrary RTE solvers, *Journal of Heat Transfer* 115 (4)  
553 (1993) 1004–1012. doi:10.1115/1.2911354.
- 554 [16] H. C. Hottel, F. Sarofim, *Radiative Transfer*, McGraw-Hill, 1967.

- 555 [17] P. Nakod, G. Krishnamoorthy, M. Sami, S. Orsino, A comparative evaluation  
556 of gray and non-gray radiation modeling strategies in oxy-coal combustion  
557 simulations, *Applied Thermal Engineering* 54 (2) (2013) 422–432. doi:  
558 10.1016/j.applthermaleng.2013.01.049.
- 559 [18] L. G. P. Rodrigues, I. M. Machado, A. Ziemniczak, F. M. Pereira, P. R.  
560 Pagot, F. H. R. França, Comparisons between numerical simulations and  
561 experimental measurements of radiative heat flux for a series of CH<sub>4</sub>/N<sub>2</sub>  
562 diluted laminar non-premixed flames, *Combustion Science and Technology*  
563 193 (1) (2021) 1–22. doi:10.1080/00102202.2019.1646733.
- 564 [19] L. D. Lemos, L. A. Q. Llanos, F. M. Pereira, F. R. Centeno, F. H. R. França,  
565 Comparison between numerical and experimental data of the radiative heat  
566 transfer in a natural gas/CO<sub>2</sub>/H<sub>2</sub> turbulent flame, *Fuel* 281 (2020) 118740.  
567 doi:10.1016/j.fuel.2020.118740.
- 568 [20] X. Cai, S. Shan, G. Jin, J. Yu, Z. Zhou, New weighted-sum-of-gray-gases  
569 radiation model for oxy-fuel combustion simulation of semi-coke from coal-  
570 based poly-generation, *Thermal Science and Engineering Progress* 46 (2023)  
571 102233. doi:https://doi.org/10.1016/j.tsep.2023.102233.
- 572 [21] G. Krishnamoorthy, A new weighted-sum-of-gray-gases model for CO<sub>2</sub>-H<sub>2</sub>O  
573 gas mixtures, *International Communications in Heat and Mass Transfer*  
574 37 (9) (2010) 1182–1186. doi:doi.org/10.1016/j.icheatmasstransfer.  
575 2010.07.007.
- 576 [22] R. Johansson, B. Leckner, K. Andersson, F. Johnsson, Account for variations  
577 in the H<sub>2</sub>O to CO<sub>2</sub> molar ratio when modelling gaseous radiative heat  
578 transfer with the weighted-sum-of-grey-gases model, *Combustion and Flame*  
579 158 (5) (2011) 893–901. doi:10.1016/j.combustflame.2011.02.001.
- 580 [23] T. Kangwanpongpan, F. H. França, R. C. da Silva, P. S. Schneider, H. J.  
581 Krautz, New correlations for the weighted-sum-of-gray-gases model in oxy-  
582 fuel conditions based on HITEMP 2010 database, *International Journal*

- 583 of Heat and Mass Transfer 55 (25) (2012) 7419–7433. doi:10.1016/j.  
584 ijheatmasstransfer.2012.07.032.
- 585 [24] L. J. Dorigon, G. Duciak, R. Brittes, F. Cassol, M. Galarça, F. H.  
586 França, WSGG correlations based on HITEMP2010 for computation of  
587 thermal radiation in non-isothermal, non-homogeneous H<sub>2</sub>O/CO<sub>2</sub> mix-  
588 tures, International Journal of Heat and Mass Transfer 64 (2013) 863–873.  
589 doi:10.1016/j.ijheatmasstransfer.2013.05.010.
- 590 [25] M. H. Bordbar, G. Weceł, T. Hyppänen, A line by line based weighted  
591 sum of gray gases model for inhomogeneous CO<sub>2</sub>-H<sub>2</sub>O mixture in oxy-fired  
592 combustion, Combustion and Flame 161 (9) (2014) 2435–2445.
- 593 [26] F. Cassol, R. Brittes, F. H. França, O. A. Ezekoye, Application of the  
594 weighted-sum-of-gray-gases model for media composed of arbitrary concen-  
595 trations of H<sub>2</sub>O, CO<sub>2</sub> and soot, International Journal of Heat and Mass  
596 Transfer 79 (2014) 796–806. doi:10.1016/j.ijheatmasstransfer.2014.  
597 08.032.
- 598 [27] R. Brittes, F. R. Centeno, A. Ziemniczak, F. H. R. França, WSGG model  
599 correlations to compute nongray radiation from carbon monoxide in com-  
600 bustion applications, Journal of Heat Transfer 139 (4) (2017) 041202.  
601 doi:10.1115/1.4035394.
- 602 [28] H. Bordbar, G. C. Fraga, S. Hostikka, An extended weighted-sum-of-gray-  
603 gases model to account for all CO<sub>2</sub>-H<sub>2</sub>O molar fraction ratios in thermal  
604 radiation, International Communications in Heat and Mass Transfer 110  
605 (2020) 104400. doi:10.1016/j.icheatmasstransfer.2019.104400.
- 606 [29] H. Sadeghi, S. Hostikka, G. C. Fraga, H. Bordbar, Weighted-sum-of-gray-  
607 gases models for non-gray thermal radiation of hydrocarbon fuel vapors,  
608 CH<sub>4</sub>, CO and soot, Fire Safety Journal 125 (2021) 103420. doi:10.1016/  
609 j.firesaf.2021.103420.

- 610 [30] A. H. B. Selhorst, G. C. Fraga, F. R. Coelho, H. Bordbar, F. H. R. França,  
611 A compact WSGG formulation to account for inhomogeneity of H<sub>2</sub>O-CO<sub>2</sub>  
612 mixtures in combustion systems, *Journal of Heat Transfer* 144 (7). doi:  
613 10.1115/1.4054239.
- 614 [31] R. J. C. Fonseca, G. C. Fraga, F. R. Coelho, F. H. R. França, A wide-  
615 band based weighted-sum-of-gray-gases model for participating media:  
616 Application to H<sub>2</sub>O-CO<sub>2</sub> mixtures with or without soot, *International*  
617 *Journal of Heat and Mass Transfer* 204 (2023) 123839. doi:10.1016/j.  
618 ijheatmasstransfer.2022.123839.
- 619 [32] J. Consalvi, F. Andre, F. Coelho, F. França, F. Nmira, M. Galtier,  
620 V. Solovjov, B. Webb, Assessment of engineering gas radiative prop-  
621 erty models in high pressure turbulent jet diffusion flames, *Journal of*  
622 *Quantitative Spectroscopy and Radiative Transfer* 253 (2020) 107169.  
623 doi:10.1016/j.jqsrt.2020.107169.
- 624 [33] V. Kez, F. Liu, J. Consalvi, J. Ströhle, B. Epple, A comprehensive evaluation  
625 of different radiation models in a gas turbine combustor under conditions of  
626 oxy-fuel combustion with dry recycle, *Journal of Quantitative Spectroscopy*  
627 *and Radiative Transfer* 172 (2016) 121–133.
- 628 [34] H. Chu, M. Gu, J.-L. Consalvi, F. Liu, H. Zhou, Effects of total pressure on  
629 non-grey gas radiation transfer in oxy-fuel combustion using the LBL, SNB,  
630 SNBCK, WSGG, and FSCK methods, *Journal of Quantitative Spectroscopy*  
631 *and Radiative Transfer* 172 (2016) 24–35.
- 632 [35] H. Chu, J.-L. Consalvi, M. Gu, F. Liu, Calculations of radiative heat transfer  
633 in an axisymmetric jet diffusion flame at elevated pressures using different  
634 gas radiation models, *Journal of Quantitative Spectroscopy and Radiative*  
635 *Transfer* 197 (2017) 12–25. doi:10.1016/j.jqsrt.2017.02.008.
- 636 [36] M. Bahador, B. Sunden, Evaluation of weighted sum of grey gases coefficients  
637 for combustion gases using predicted emissivities from high resolution

- 638 spectroscopic databases, in: Proceedings of ASME Turbo Expo 2008; Power  
639 for Land, Sea and Air, ASMEDC, 2008. doi:10.1115/gt2008-51028.
- 640 [37] S. Shan, B. Qian, Z. Zhou, Z. Wang, K. Cen, New pressurized WSGG  
641 model and the effect of pressure on the radiation heat transfer of H<sub>2</sub>O/CO<sub>2</sub>  
642 gas mixtures, International Journal of Heat and Mass Transfer 121 (2018)  
643 999–1010. doi:10.1016/j.ijheatmasstransfer.2018.01.079.
- 644 [38] C. Paul, S. F. Fernandez, D. C. Haworth, S. Roy, M. F. Modest, A detailed  
645 modeling study of radiative heat transfer in a heavy-duty diesel engine, Com-  
646 bustion and Flame 200 (2019) 325–341. doi:10.1016/j.combustflame.  
647 2018.11.032.
- 648 [39] A. Johnson, S. Zhang, X. Zhao, Wide-band models for high-pressure engine  
649 conditions, in: AIAA Propulsion and Energy 2020 Forum, American Institute  
650 of Aeronautics and Astronautics, 2020.
- 651 [40] J. T. Pearson, B. W. Webb, V. P. Solovjov, J. Ma, Effect of total pressure  
652 on the absorption line blackbody distribution function and radiative transfer  
653 in H<sub>2</sub>O, CO<sub>2</sub>, and CO, Journal of Quantitative Spectroscopy and Radiative  
654 Transfer 143 (2014) 100–110. doi:10.1016/j.jqsrt.2013.08.011.
- 655 [41] J. T. Pearson, B. W. Webb, V. P. Solovjov, J. Ma, Efficient representation  
656 of the absorption line blackbody distribution function for H<sub>2</sub>O, CO<sub>2</sub>, and  
657 CO at variable temperature, mole fraction, and total pressure, Journal  
658 of Quantitative Spectroscopy and Radiative Transfer 138 (2014) 82–96.  
659 doi:10.1016/j.jqsrt.2014.01.019.
- 660 [42] J. Cai, M. F. Modest, Improved full-spectrum *k*-distribution implemen-  
661 tation for inhomogeneous media using a narrow-band database, Journal  
662 of Quantitative Spectroscopy and Radiative Transfer 141 (2014) 65–72.  
663 doi:10.1016/j.jqsrt.2014.02.028.
- 664 [43] H. Chu, F. Ren, Y. Feng, M. Gu, S. Zheng, A comprehensive evaluation  
665 of the non gray gas thermal radiation using the line-by-line model in one-

- 666 and two-dimensional enclosures, Applied Thermal Engineering 124 (2017)  
667 362–370. doi:10.1016/j.applthermaleng.2017.06.037.
- 668 [44] Y. Zhou, C. Wang, T. Ren, A machine learning based efficient and compact  
669 full-spectrum correlated  $k$ -distribution model, Journal of Quantitative Spectroscopy and Radiative Transfer 254 (2020) 107199. doi:  
670 10.1016/j.jqsrt.2020.107199.  
671
- 672 [45] Y. Liu, J. Zhu, G. Liu, F. Liu, J.-L. Consalvi, Assessment of various full-  
673 spectrum correlated  $k$ -distribution methods in radiative heat transfer in  
674 oxy-fuel sooting flames, International Journal of Thermal Sciences 184 (2023)  
675 107919. doi:10.1016/j.ijthermalsci.2022.107919.
- 676 [46] F. R. Centeno, R. Brittes, L. G. Rodrigues, F. R. Coelho, F. H. França,  
677 Evaluation of the WSGG model against line-by-line calculation of thermal  
678 radiation in a non-gray sooting medium representing an axisymmetric  
679 laminar jet flame, International Journal of Heat and Mass Transfer 124  
680 (2018) 475–483. doi:10.1016/j.ijheatmasstransfer.2018.02.040.
- 681 [47] K. D. Lathrop, B. G. Carlson, Discrete ordinates angular quadrature of the  
682 neutron transport equation doi:10.2172/4666281.
- 683 [48] O. Marin, R. Buckius, A simplified wide band model of the cumulative  
684 distribution function for water vapor, International Journal of Heat and  
685 Mass Transfer 41 (19) (1998) 2877–2892. doi:10.1016/s0017-9310(98)  
686 00033-7.
- 687 [49] R. J. C. Fonseca, G. C. Fraga, F. H. R. França, Comparison of the perfor-  
688 mances of the wide-band based weighted-sum-of-gray-gases and box models  
689 in the calculation of non-gray boundaries at high pressures, in: Proceedings  
690 of the 27th International Congress of Mechanical Engineering, ABCM, 2023.
- 691 **5. Appendix A - WBW correlations for the mixture of H<sub>2</sub>O and CO<sub>2</sub>**

Table 5: One gray gas per spectral band and  $p = 10$  atm.

$j$	$\kappa_{p,j}$ [atm $^{-1}$ m $^{-1}$ ]	$b_{j,0}$	$b_{j,1}$ [K $^{-1}$ ]	$b_{j,2}$ [K $^{-2}$ ]	$b_{j,3}$ [K $^{-3}$ ]	$b_{j,4}$ [K $^{-4}$ ]	$b_{j,5}$ [K $^{-5}$ ]
Band 1							
1	41.266	$7.854 \times 10^{-1}$	$3.450 \times 10^{-4}$	$-2.651 \times 10^{-7}$	$1.104 \times 10^{-10}$	$-2.216 \times 10^{-14}$	$1.542 \times 10^{-18}$
Band 2							
1	16.541	$4.041 \times 10^{-1}$	$2.075 \times 10^{-3}$	$-2.873 \times 10^{-6}$	$1.886 \times 10^{-9}$	$-5.926 \times 10^{-13}$	$7.180 \times 10^{-17}$
Band 3							
1	4.747	$6.441 \times 10^{-1}$	$1.606 \times 10^{-4}$	$2.953 \times 10^{-7}$	$-3.252 \times 10^{-10}$	$1.206 \times 10^{-13}$	$-1.572 \times 10^{-17}$
Band 4							
1	1.731	$-2.616 \times 10^{-1}$	$2.023 \times 10^{-3}$	$-1.720 \times 10^{-6}$	$8.813 \times 10^{-10}$	$-2.469 \times 10^{-13}$	$2.853 \times 10^{-17}$
Band 5							
1	0.664	$-2.664 \times 10^{-1}$	$1.483 \times 10^{-3}$	$-8.428 \times 10^{-7}$	$1.764 \times 10^{-10}$	$8.476 \times 10^{-15}$	$-5.820 \times 10^{-18}$

Table 6: Two gray gases per spectral band and  $p = 10$  atm.

$j$	$\kappa_{p,j}$ [atm $^{-1}$ m $^{-1}$ ]	$b_{j,0}$	$b_{j,1}$ [K $^{-1}$ ]	$b_{j,2}$ [K $^{-2}$ ]	$b_{j,3}$ [K $^{-3}$ ]	$b_{j,4}$ [K $^{-4}$ ]	$b_{j,5}$ [K $^{-5}$ ]
Band 1							
1	6.392	$5.901 \times 10^{-2}$	$2.168 \times 10^{-3}$	$-3.340 \times 10^{-6}$	$2.207 \times 10^{-9}$	$-6.967 \times 10^{-13}$	$8.536 \times 10^{-17}$
2	157.314	$7.202 \times 10^{-1}$	$-1.578 \times 10^{-3}$	$2.688 \times 10^{-6}$	$-1.838 \times 10^{-9}$	$5.923 \times 10^{-13}$	$-7.370 \times 10^{-17}$
Band 2							
1	4.098	$6.541 \times 10^{-1}$	$-3.377 \times 10^{-4}$	$-4.406 \times 10^{-9}$	$1.812 \times 10^{-10}$	$-9.021 \times 10^{-14}$	$1.397 \times 10^{-17}$
2	92.060	$1.598 \times 10^{-1}$	$6.770 \times 10^{-4}$	$1.049 \times 10^{-8}$	$-5.070 \times 10^{-10}$	$2.902 \times 10^{-13}$	$-4.916 \times 10^{-17}$
Band 3							
1	0.845	$8.045 \times 10^{-1}$	$-3.996 \times 10^{-4}$	$2.591 \times 10^{-9}$	$1.535 \times 10^{-10}$	$-7.461 \times 10^{-14}$	$1.122 \times 10^{-17}$
2	21.998	$-7.505 \times 10^{-2}$	$6.427 \times 10^{-4}$	$-2.700 \times 10^{-9}$	$-2.203 \times 10^{-10}$	$9.986 \times 10^{-14}$	$-1.401 \times 10^{-17}$
Band 4							
1	0.363	$5.602 \times 10^{-2}$	$3.526 \times 10^{-4}$	$-1.083 \times 10^{-9}$	$-5.686 \times 10^{-11}$	$1.464 \times 10^{-15}$	$3.522 \times 10^{-18}$
2	3.909	$-9.346 \times 10^{-2}$	$7.268 \times 10^{-4}$	$5.016 \times 10^{-9}$	$-4.115 \times 10^{-10}$	$2.324 \times 10^{-13}$	$-3.910 \times 10^{-17}$
Band 5							
1	0.228	$6.727 \times 10^{-2}$	$2.462 \times 10^{-4}$	$-3.665 \times 10^{-10}$	$9.784 \times 10^{-11}$	$-8.077 \times 10^{-14}$	$1.577 \times 10^{-17}$
2	2.606	$-1.917 \times 10^{-1}$	$7.385 \times 10^{-4}$	$8.323 \times 10^{-10}$	$-4.999 \times 10^{-10}$	$2.753 \times 10^{-13}$	$-4.467 \times 10^{-17}$



Table 7: Three gray gases per spectral band and  $p = 10$  atm.

$j$	$\kappa_{p,j}$ [atm $^{-1}$ m $^{-1}$ ]	$b_{j,0}$	$b_{j,1}$ [K $^{-1}$ ]	$b_{j,2}$ [K $^{-2}$ ]	$b_{j,3}$ [K $^{-3}$ ]	$b_{j,4}$ [K $^{-4}$ ]	$b_{j,5}$ [K $^{-5}$ ]
Band 1							
1	2.014	$4.670 \times 10^{-1}$	$-9.185 \times 10^{-5}$	$1.319 \times 10^{-8}$	$-2.965 \times 10^{-10}$	$2.052 \times 10^{-13}$	$-3.818 \times 10^{-17}$
2	20.292	$-1.696 \times 10^{-1}$	$5.197 \times 10^{-4}$	$-1.357 \times 10^{-8}$	$1.316 \times 10^{-11}$	$-5.893 \times 10^{-14}$	$1.571 \times 10^{-17}$
3	224.620	$5.975 \times 10^{-1}$	$-2.403 \times 10^{-4}$	$3.009 \times 10^{-9}$	$1.272 \times 10^{-10}$	$-5.424 \times 10^{-14}$	$6.696 \times 10^{-18}$
Band 2							
1	1.147	$6.228 \times 10^{-1}$	$-6.781 \times 10^{-4}$	$-7.712 \times 10^{-9}$	$4.817 \times 10^{-10}$	$-2.716 \times 10^{-13}$	$4.521 \times 10^{-17}$
2	17.902	$-1.525 \times 10^{-1}$	$1.064 \times 10^{-3}$	$1.099 \times 10^{-8}$	$-8.322 \times 10^{-10}$	$4.869 \times 10^{-13}$	$-8.262 \times 10^{-17}$
3	283.831	$3.998 \times 10^{-1}$	$-1.273 \times 10^{-4}$	$1.886 \times 10^{-9}$	$8.779 \times 10^{-11}$	$-5.184 \times 10^{-14}$	$8.386 \times 10^{-18}$
Band 3							
1	0.499	$4.501 \times 10^{-1}$	$1.295 \times 10^{-4}$	$1.026 \times 10^{-8}$	$-3.750 \times 10^{-10}$	$2.378 \times 10^{-13}$	$-4.235 \times 10^{-17}$
2	4.182	$5.893 \times 10^{-1}$	$-8.119 \times 10^{-4}$	$-1.349 \times 10^{-8}$	$8.691 \times 10^{-10}$	$-5.170 \times 10^{-13}$	$8.895 \times 10^{-17}$
3	40.812	$-2.982 \times 10^{-1}$	$9.740 \times 10^{-4}$	$4.459 \times 10^{-9}$	$-6.283 \times 10^{-10}$	$3.456 \times 10^{-13}$	$-5.658 \times 10^{-17}$
Band 4							
1	0.256	$2.923 \times 10^{-2}$	$5.495 \times 10^{-4}$	$-1.409 \times 10^{-9}$	$-3.188 \times 10^{-10}$	$1.464 \times 10^{-13}$	$-1.951 \times 10^{-17}$
2	1.981	$6.897 \times 10^{-3}$	$1.939 \times 10^{-5}$	$2.546 \times 10^{-9}$	$2.818 \times 10^{-10}$	$-1.573 \times 10^{-13}$	$2.443 \times 10^{-17}$
3	7.826	$-7.555 \times 10^{-2}$	$6.006 \times 10^{-4}$	$2.593 \times 10^{-9}$	$-5.085 \times 10^{-10}$	$2.844 \times 10^{-13}$	$-4.643 \times 10^{-17}$
Band 5							
1	0.156	$7.447 \times 10^{-2}$	$3.432 \times 10^{-4}$	$7.255 \times 10^{-10}$	$-5.547 \times 10^{-11}$	$9.338 \times 10^{-15}$	$8.150 \times 10^{-19}$
2	1.359	$-9.669 \times 10^{-2}$	$2.901 \times 10^{-4}$	$-1.427 \times 10^{-9}$	$-5.856 \times 10^{-12}$	$-1.196 \times 10^{-14}$	$3.132 \times 10^{-18}$
3	6.375	$-9.131 \times 10^{-2}$	$4.255 \times 10^{-4}$	$1.561 \times 10^{-9}$	$-3.923 \times 10^{-10}$	$2.243 \times 10^{-13}$	$-3.704 \times 10^{-17}$

Table 8: Four gray gases per spectral band and  $p = 10$  atm.

$j$	$K_{p,j}$ [atm $^{-1}$ m $^{-1}$ ]	$b_{j,0}$	$b_{j,1}$ [K $^{-1}$ ]	$b_{j,2}$ [K $^{-2}$ ]	$b_{j,3}$ [K $^{-3}$ ]	$b_{j,4}$ [K $^{-4}$ ]	$b_{j,5}$ [K $^{-5}$ ]
Band 1							
1	1.115	$8.967 \times 10^{-2}$	$1.775 \times 10^{-3}$	$-3.907 \times 10^{-6}$	$3.099 \times 10^{-9}$	$-1.083 \times 10^{-12}$	$1.409 \times 10^{-16}$
2	7.801	$-1.398 \times 10^{-1}$	$-1.087 \times 10^{-5}$	$1.887 \times 10^{-6}$	$-2.121 \times 10^{-9}$	$8.476 \times 10^{-13}$	$-1.179 \times 10^{-16}$
3	50.238	$4.066 \times 10^{-1}$	$-8.260 \times 10^{-4}$	$5.938 \times 10^{-7}$	$7.842 \times 10^{-11}$	$-1.270 \times 10^{-13}$	$2.368 \times 10^{-17}$
4	287.062	$4.317 \times 10^{-1}$	$-1.413 \times 10^{-4}$	$3.175 \times 10^{-7}$	$-3.273 \times 10^{-10}$	$1.320 \times 10^{-13}$	$-1.866 \times 10^{-17}$
Band 2							
1	0.747	1.320	$-4.071 \times 10^{-3}$	$5.269 \times 10^{-6}$	$-3.290 \times 10^{-9}$	$9.978 \times 10^{-13}$	$-1.181 \times 10^{-16}$
2	6.831	-1.067	$5.025 \times 10^{-3}$	$-6.677 \times 10^{-6}$	$4.107 \times 10^{-9}$	$-1.203 \times 10^{-12}$	$1.368 \times 10^{-16}$
3	40.984	$3.252 \times 10^{-1}$	$-3.695 \times 10^{-4}$	$6.907 \times 10^{-7}$	$-3.678 \times 10^{-10}$	$6.940 \times 10^{-14}$	$-2.934 \times 10^{-18}$
4	447.002	$1.060 \times 10^{-1}$	$6.741 \times 10^{-4}$	$-1.109 \times 10^{-6}$	$7.760 \times 10^{-10}$	$-2.531 \times 10^{-13}$	$3.135 \times 10^{-17}$
Band 3							
1	0.379	$-3.354 \times 10^{-1}$	$3.071 \times 10^{-3}$	$-4.630 \times 10^{-6}$	$3.070 \times 10^{-9}$	$-9.641 \times 10^{-13}$	$1.167 \times 10^{-16}$
2	2.047	1.289	$-3.609 \times 10^{-3}$	$4.670 \times 10^{-6}$	$-2.863 \times 10^{-9}$	$8.486 \times 10^{-13}$	$-9.773 \times 10^{-17}$
3	14.672	$3.292 \times 10^{-2}$	$-3.221 \times 10^{-4}$	$9.697 \times 10^{-7}$	$-7.204 \times 10^{-10}$	$2.462 \times 10^{-13}$	$-3.228 \times 10^{-17}$
4	73.427	$-3.460 \times 10^{-1}$	$1.639 \times 10^{-3}$	$-1.766 \times 10^{-6}$	$9.204 \times 10^{-10}$	$-2.472 \times 10^{-13}$	$2.695 \times 10^{-17}$
Band 4							
1	0.199	$1.876 \times 10^{-1}$	$-3.719 \times 10^{-4}$	$1.711 \times 10^{-6}$	$-1.710 \times 10^{-9}$	$6.511 \times 10^{-13}$	$-8.725 \times 10^{-17}$
2	1.106	$-1.890 \times 10^{-1}$	$1.387 \times 10^{-3}$	$-2.684 \times 10^{-6}$	$2.325 \times 10^{-9}$	$-8.638 \times 10^{-13}$	$1.165 \times 10^{-16}$
3	3.813	$6.175 \times 10^{-2}$	$-6.448 \times 10^{-4}$	$2.079 \times 10^{-6}$	$-1.780 \times 10^{-9}$	$6.434 \times 10^{-13}$	$-8.532 \times 10^{-17}$
4	14.267	$-2.349 \times 10^{-1}$	$1.462 \times 10^{-3}$	$-2.129 \times 10^{-6}$	$1.382 \times 10^{-9}$	$-4.298 \times 10^{-13}$	$5.183 \times 10^{-17}$
Band 5							
1	0.126	$1.818 \times 10^{-1}$	$-1.182 \times 10^{-4}$	$7.569 \times 10^{-7}$	$-5.984 \times 10^{-10}$	$1.832 \times 10^{-13}$	$-1.987 \times 10^{-17}$
2	0.915	$-2.280 \times 10^{-1}$	$1.034 \times 10^{-3}$	$-1.407 \times 10^{-6}$	$1.014 \times 10^{-9}$	$-3.341 \times 10^{-13}$	$4.077 \times 10^{-17}$
3	2.921	$1.129 \times 10^{-1}$	$-6.657 \times 10^{-4}$	$1.707 \times 10^{-6}$	$-1.427 \times 10^{-9}$	$4.979 \times 10^{-13}$	$-6.331 \times 10^{-17}$
4	12.553	$-2.161 \times 10^{-1}$	$1.060 \times 10^{-3}$	$-1.454 \times 10^{-6}$	$8.836 \times 10^{-10}$	$-2.535 \times 10^{-13}$	$2.811 \times 10^{-17}$

Table 9: One gray gas per spectral band and  $p = 20$  atm.

$j$	$\kappa_{p,j}$ [atm $^{-1}$ m $^{-1}$ ]	$b_{j,0}$	$b_{j,1}$ [K $^{-1}$ ]	$b_{j,2}$ [K $^{-2}$ ]	$b_{j,3}$ [K $^{-3}$ ]	$b_{j,4}$ [K $^{-4}$ ]	$b_{j,5}$ [K $^{-5}$ ]
Band 1							
1	73.822	1.002	$-5.479 \times 10^{-4}$	$1.114 \times 10^{-6}$	$-8.714 \times 10^{-10}$	$3.050 \times 10^{-13}$	$-3.985 \times 10^{-17}$
Band 2							
1	38.922	$2.952 \times 10^{-1}$	$2.456 \times 10^{-3}$	$-3.376 \times 10^{-6}$	$2.222 \times 10^{-9}$	$-7.038 \times 10^{-13}$	$8.622 \times 10^{-17}$
Band 3							
1	6.632	$6.839 \times 10^{-1}$	$2.325 \times 10^{-4}$	$2.184 \times 10^{-7}$	$-3.291 \times 10^{-10}$	$1.402 \times 10^{-13}$	$-2.012 \times 10^{-17}$
Band 4							
1	3.048	$-1.815 \times 10^{-1}$	$1.633 \times 10^{-3}$	$-9.796 \times 10^{-7}$	$3.188 \times 10^{-10}$	$-5.815 \times 10^{-14}$	$4.999 \times 10^{-18}$
Band 5							
1	0.957	$-1.735 \times 10^{-1}$	$1.157 \times 10^{-3}$	$-3.362 \times 10^{-7}$	$-1.421 \times 10^{-10}$	$1.015 \times 10^{-13}$	$-1.623 \times 10^{-17}$

Table 10: Two gray gases per spectral band and  $p = 20$  atm.

$j$	$\kappa_{p,j}$ [atm $^{-1}$ m $^{-1}$ ]	$b_{j,0}$	$b_{j,1}$ [K $^{-1}$ ]	$b_{j,2}$ [K $^{-2}$ ]	$b_{j,3}$ [K $^{-3}$ ]	$b_{j,4}$ [K $^{-4}$ ]	$b_{j,5}$ [K $^{-5}$ ]
Band 1							
1	8.634	$2.545 \times 10^{-1}$	$1.603 \times 10^{-3}$	$-2.758 \times 10^{-6}$	$1.869 \times 10^{-9}$	$-5.902 \times 10^{-13}$	$7.165 \times 10^{-17}$
2	280.661	$7.556 \times 10^{-1}$	$-1.955 \times 10^{-3}$	$3.534 \times 10^{-6}$	$-2.506 \times 10^{-9}$	$8.199 \times 10^{-13}$	$-1.022 \times 10^{-16}$
Band 2							
1	6.968	1.012	$-1.877 \times 10^{-3}$	$2.320 \times 10^{-6}$	$-1.435 \times 10^{-9}$	$4.401 \times 10^{-13}$	$-5.266 \times 10^{-17}$
2	216.256	$-6.075 \times 10^{-1}$	$4.066 \times 10^{-3}$	$-5.364 \times 10^{-6}$	$3.451 \times 10^{-9}$	$-1.081 \times 10^{-12}$	$1.313 \times 10^{-16}$
Band 3							
1	1.471	$2.030 \times 10^{-2}$	$2.394 \times 10^{-3}$	$-3.601 \times 10^{-6}$	$2.356 \times 10^{-9}$	$-7.291 \times 10^{-13}$	$8.725 \times 10^{-17}$
2	38.094	$6.177 \times 10^{-1}$	$-1.737 \times 10^{-3}$	$3.157 \times 10^{-6}$	$-2.242 \times 10^{-9}$	$7.298 \times 10^{-13}$	$-9.043 \times 10^{-17}$
Band 4							
1	0.459	$3.043 \times 10^{-1}$	$-7.953 \times 10^{-4}$	$2.024 \times 10^{-6}$	$-1.659 \times 10^{-9}$	$5.711 \times 10^{-13}$	$-7.165 \times 10^{-17}$
2	6.685	$-4.011 \times 10^{-1}$	$2.161 \times 10^{-3}$	$-2.439 \times 10^{-6}$	$1.529 \times 10^{-9}$	$-4.758 \times 10^{-13}$	$5.738 \times 10^{-17}$
Band 5							
1	0.264	$2.481 \times 10^{-1}$	$-4.124 \times 10^{-4}$	$9.903 \times 10^{-7}$	$-6.056 \times 10^{-10}$	$1.543 \times 10^{-13}$	$-1.406 \times 10^{-17}$
2	4.131	$-3.257 \times 10^{-1}$	$1.347 \times 10^{-3}$	$-9.666 \times 10^{-7}$	$2.646 \times 10^{-10}$	$-5.653 \times 10^{-15}$	$-6.105 \times 10^{-18}$

Table 11: Three gray gases per spectral band and  $p = 20$  atm.

$j$	$\kappa_{p,j}$ [atm $^{-1}$ m $^{-1}$ ]	$b_{j,0}$	$b_{j,1}$ [K $^{-1}$ ]	$b_{j,2}$ [K $^{-2}$ ]	$b_{j,3}$ [K $^{-3}$ ]	$b_{j,4}$ [K $^{-4}$ ]	$b_{j,5}$ [K $^{-5}$ ]
Band 1							
1	3.100	$-3.928 \times 10^{-1}$	$4.392 \times 10^{-3}$	$-7.835 \times 10^{-6}$	$5.747 \times 10^{-9}$	$-1.926 \times 10^{-12}$	$2.438 \times 10^{-16}$
2	29.327	1.268	$-6.301 \times 10^{-3}$	$1.128 \times 10^{-5}$	$-8.435 \times 10^{-9}$	$2.865 \times 10^{-12}$	$-3.656 \times 10^{-16}$
3	372.427	$8.544 \times 10^{-2}$	$1.957 \times 10^{-3}$	$-3.391 \times 10^{-6}$	$2.592 \times 10^{-9}$	$-8.925 \times 10^{-13}$	$1.147 \times 10^{-16}$
Band 2							
1	1.937	1.328	$-3.644 \times 10^{-3}$	$4.345 \times 10^{-6}$	$-2.539 \times 10^{-9}$	$7.312 \times 10^{-13}$	$-8.301 \times 10^{-17}$
2	26.597	-1.162	$4.990 \times 10^{-3}$	$-5.822 \times 10^{-6}$	$3.299 \times 10^{-9}$	$-9.175 \times 10^{-13}$	$1.011 \times 10^{-16}$
3	375.122	$3.705 \times 10^{-1}$	$4.399 \times 10^{-4}$	$-1.088 \times 10^{-6}$	$9.794 \times 10^{-10}$	$-3.764 \times 10^{-13}$	$5.189 \times 10^{-17}$
Band 3							
1	0.718	$-5.613 \times 10^{-1}$	$3.357 \times 10^{-3}$	$-4.260 \times 10^{-6}$	$2.428 \times 10^{-9}$	$-6.684 \times 10^{-13}$	$7.218 \times 10^{-17}$
2	5.355	1.159	$-2.431 \times 10^{-3}$	$2.307 \times 10^{-6}$	$-9.089 \times 10^{-10}$	$1.450 \times 10^{-13}$	$-4.608 \times 10^{-18}$
3	69.433	$-1.304 \times 10^{-2}$	$-2.726 \times 10^{-5}$	$1.231 \times 10^{-6}$	$-1.264 \times 10^{-9}$	$4.900 \times 10^{-13}$	$-6.759 \times 10^{-17}$
Band 4							
1	0.300	$3.812 \times 10^{-1}$	$-1.253 \times 10^{-3}$	$3.255 \times 10^{-6}$	$-2.919 \times 10^{-9}$	$1.076 \times 10^{-12}$	$-1.426 \times 10^{-16}$
2	2.358	$-2.019 \times 10^{-1}$	$1.228 \times 10^{-3}$	$-2.437 \times 10^{-6}$	$2.290 \times 10^{-9}$	$-8.916 \times 10^{-13}$	$1.234 \times 10^{-16}$
3	11.186	$-2.251 \times 10^{-1}$	$1.195 \times 10^{-3}$	$-7.200 \times 10^{-7}$	$1.908 \times 10^{-11}$	$9.303 \times 10^{-14}$	$-1.982 \times 10^{-17}$
Band 5							
1	0.193	$2.612 \times 10^{-1}$	$-3.730 \times 10^{-4}$	$1.113 \times 10^{-6}$	$-8.438 \times 10^{-10}$	$2.635 \times 10^{-13}$	$-2.972 \times 10^{-17}$
2	1.795	$-1.154 \times 10^{-1}$	$4.219 \times 10^{-4}$	$-3.999 \times 10^{-7}$	$3.535 \times 10^{-10}$	$-1.364 \times 10^{-13}$	$1.811 \times 10^{-17}$
3	9.054	$-1.939 \times 10^{-1}$	$8.593 \times 10^{-4}$	$-5.451 \times 10^{-7}$	$2.876 \times 10^{-12}$	$7.621 \times 10^{-14}$	$-1.557 \times 10^{-17}$

Table 12: Four gray gases per spectral band and  $p = 20$  atm.

$j$	$K_{p,j}$ [atm $^{-1}$ m $^{-1}$ ]	$b_{j,0}$	$b_{j,1}$ [K $^{-1}$ ]	$b_{j,2}$ [K $^{-2}$ ]	$b_{j,3}$ [K $^{-3}$ ]	$b_{j,4}$ [K $^{-4}$ ]	$b_{j,5}$ [K $^{-5}$ ]
Band 1							
1	2.083	$-4.887 \times 10^{-1}$	$4.612 \times 10^{-3}$	$-8.404 \times 10^{-6}$	$6.302 \times 10^{-9}$	$-2.145 \times 10^{-12}$	$2.743 \times 10^{-16}$
2	17.146	1.294	$-6.338 \times 10^{-3}$	$1.175 \times 10^{-5}$	$-9.132 \times 10^{-9}$	$3.179 \times 10^{-12}$	$-4.124 \times 10^{-16}$
3	124.311	$-2.302 \times 10^{-1}$	$2.372 \times 10^{-3}$	$-4.542 \times 10^{-6}$	$3.790 \times 10^{-9}$	$-1.374 \times 10^{-12}$	$1.827 \times 10^{-16}$
4	723.996	$3.752 \times 10^{-1}$	$-5.112 \times 10^{-4}$	$1.071 \times 10^{-6}$	$-9.195 \times 10^{-10}$	$3.377 \times 10^{-13}$	$-4.532 \times 10^{-17}$
Band 2							
1	1.457	1.438	$-4.181 \times 10^{-3}$	$5.005 \times 10^{-6}$	$-2.905 \times 10^{-9}$	$8.270 \times 10^{-13}$	$-9.273 \times 10^{-17}$
2	14.456	-1.132	$4.609 \times 10^{-3}$	$-5.380 \times 10^{-6}$	$2.955 \times 10^{-9}$	$-7.822 \times 10^{-13}$	$8.144 \times 10^{-17}$
3	89.403	$1.231 \times 10^{-1}$	$8.936 \times 10^{-4}$	$-1.370 \times 10^{-6}$	$1.085 \times 10^{-9}$	$-4.036 \times 10^{-13}$	$5.550 \times 10^{-17}$
4	1171.769	$1.406 \times 10^{-1}$	$3.536 \times 10^{-4}$	$-6.826 \times 10^{-7}$	$5.237 \times 10^{-10}$	$-1.807 \times 10^{-13}$	$2.315 \times 10^{-17}$
Band 3							
1	0.533	$-1.657 \times 10^{-1}$	$1.241 \times 10^{-3}$	$-1.082 \times 10^{-6}$	$2.364 \times 10^{-10}$	$5.073 \times 10^{-14}$	$-1.827 \times 10^{-17}$
2	2.919	$-3.331 \times 10^{-2}$	$2.397 \times 10^{-3}$	$-4.465 \times 10^{-6}$	$3.510 \times 10^{-9}$	$-1.248 \times 10^{-12}$	$1.656 \times 10^{-16}$
3	20.835	1.523	$-5.680 \times 10^{-3}$	$8.210 \times 10^{-6}$	$-5.438 \times 10^{-9}$	$1.731 \times 10^{-12}$	$-2.128 \times 10^{-16}$
4	127.066	$-7.164 \times 10^{-1}$	$2.844 \times 10^{-3}$	$-3.209 \times 10^{-6}$	$1.804 \times 10^{-9}$	$-5.141 \times 10^{-13}$	$5.836 \times 10^{-17}$
Band 4							
1	0.221	$5.365 \times 10^{-1}$	$-2.164 \times 10^{-3}$	$4.884 \times 10^{-6}$	$-4.232 \times 10^{-9}$	$1.555 \times 10^{-12}$	$-2.071 \times 10^{-16}$
2	1.190	$-3.967 \times 10^{-1}$	$2.422 \times 10^{-3}$	$-4.397 \times 10^{-6}$	$3.637 \times 10^{-9}$	$-1.340 \times 10^{-12}$	$1.811 \times 10^{-16}$
3	5.919	$2.498 \times 10^{-1}$	$-1.426 \times 10^{-3}$	$3.051 \times 10^{-6}$	$-2.343 \times 10^{-9}$	$8.174 \times 10^{-13}$	$-1.073 \times 10^{-16}$
4	21.138	$-3.572 \times 10^{-1}$	$1.974 \times 10^{-3}$	$-2.693 \times 10^{-6}$	$1.698 \times 10^{-9}$	$-5.242 \times 10^{-13}$	$6.337 \times 10^{-17}$
Band 5							
1	0.156	$4.093 \times 10^{-1}$	$-9.841 \times 10^{-4}$	$2.062 \times 10^{-6}$	$-1.524 \times 10^{-9}$	$4.851 \times 10^{-13}$	$-5.665 \times 10^{-17}$
2	1.015	$-3.268 \times 10^{-1}$	$1.440 \times 10^{-3}$	$-2.107 \times 10^{-6}$	$1.544 \times 10^{-9}$	$-5.154 \times 10^{-13}$	$6.371 \times 10^{-17}$
3	4.149	$2.092 \times 10^{-1}$	$-1.000 \times 10^{-3}$	$2.105 \times 10^{-6}$	$-1.614 \times 10^{-9}$	$5.413 \times 10^{-13}$	$-6.732 \times 10^{-17}$
4	17.376	$-2.649 \times 10^{-1}$	$1.197 \times 10^{-3}$	$-1.454 \times 10^{-6}$	$7.904 \times 10^{-10}$	$-2.056 \times 10^{-13}$	$2.083 \times 10^{-17}$