ACCURACY OF ENGINEERING METHODS FOR RADIATIVE TRANSFER IN CO2-H2O MIXTURES AT HIGH TEMPERATURE

Frédéric André, Felipe Coelho, Jean-Louis Consalvi, Francis Henrique Ramos Franca, Mathieu Galtier, Fatiha Nmira, Vladimir Solovjov, Brent Webb

ACCURACY OF ENGINEERING METHODS FOR RADIATIVE TRANSFER IN CO_2-H_2O MIXTURES AT HIGH TEMPERATURE

Frédéric ANDRE[1*], Felipe COELHO[2], Jean-Louis CONSALVI[3], Francis FRANCA[2], Mathieu GALTIER[1] , Fatiha NMIRA[4], Vladimir P. SOLOVJOV[5], Brent W. WEBB[5]

[1]Univ Lyon, CNRS, INSA-Lyon, Université Claude Bernard Lyon 1, CETHIL UMR5008, F-69621 Villeurbanne, France
[2]ME Department, Federal University of Rio Grande do Sul, Porto Alegre, RS, Brazil
[3]Aix-Marseille Université, IUSTI/ UMR CNRS 7343, 5 rue E. Fermi, 13453 Marseille, France
[4]Direction R&D EDF, 6 quai Watier, 78400 Chatou, France
[5]Brigham Young University, 360G EB, Provo, UT 84602, USA

ABSTRACT. The aim of the paper is to evaluate a set of recently proposed engineering methods of gas radiation. For this purpose, a 3D stochastic ray tracing code was developed to treat realistic geometries. Model parameters based on the same LBL dataset were constructed for all approximate methods. Comparisons consist of two steps: 1/ a set of rays randomly spread over the unit sphere is chosen and narrow band models are assessed against LBL calculations. The most accurate narrow band method is chosen as the reference, 2/ all models are then compared with the chosen reference. For the cases considered in this paper, it was found that: 1/ the ℓ-distribution approach is more accurate than C*k* methods and can be used as the reference; 2/ the RC-SLW model provides very accurate predictions; 3/ the WSGG technique, which is the fastest method considered in this work, provides acceptable estimations, even in highly non-isothermal situations.

1. INTRODUCTION

The goal of the present paper is to describe the current stage of development of a chain of codes to compare approximate models of gas radiation with LBL reference calculations in 3D realistic geometries. The objective of this analysis is not to suggest any kind of best model but to propose a fair comparison of a set of engineering methods of gas radiation in high temperature media, from the simplest one, the WSGG, up to the most recent techniques. We only consider models whose parameters are directly derived from LBL data.

Several usual techniques, such as the widely used narrow band C*k* or Weighted-Sum-of-Gray-Gases models, are thus considered. Other methods proposed recently such as the RC-SLW model [1] or the ℓ-distribution approach [2] are also studied. All the approximate models described in this work use coefficients based on the same initial LBL database. This allows focusing on the intrinsic accuracy of the models, not on how their parameters were generated. Evaluations are founded on a stochastic ray tracing method that generates ray paths used to compare the approximate models over the same sequences of non-uniform sub-paths. Accordingly, even if the calculations are not converged, i.e., if the number of rays is not sufficient to ensure a proper estimate of quantities of interest such as the radiative heat flux or the radiative power, the analysis provides a statistically relevant test of accuracy

* Corresponding Author: frederic.andre@insa-lyon.fr.

of the spectral models against a given chosen reference. This reference can be a LBL calculation, for small number of rays, or any other possible model, for larger ones.

One of the main originalities of the work is that it involves several teams who usually use their own LBL datasets to produce approximate models. Here, the same high resolution spectra were used as inputs by all partners. Furthermore, to the best of the authors' knowledge, this work describes the first evaluation of the Godson-Weinreb-Neuendorffer (GWN) method [3] to treat non-uniform paths in realistic radiative heat transfer problems. Its application is made here within the frame of the ℓ-distribution approach. It is shown to provide a realistic alternative to more established techniques such as C*k* models, at a fraction of their computational cost.

2. METHODOLOGY

The comparison's strategy is founded on a 3D stochastic ray tracing code developed specifically for this purpose. It allows choosing particular locations inside a given 3D grid at which a prescribed number of rays (1,000 and 100,000 rays were studied here) randomly spread over the unit sphere are chosen. Then, a ray tracing method is used to solve the radiative transfer problem over the corresponding set of rays. The same sequences of random numbers are used for the generation of the non-uniform paths treated by all approximate methods of gas radiation allowing a direct evaluation of the techniques, even for small number of rays. Indeed, even if the radiative calculation is not statistically converged, the use of the same paths ensures a fair comparison of the various approximate methods of gas radiation. Spectral integration is performed deterministically for all models. The code can treat configurations involving non-gray boundaries, but this option is not used here. Furthermore, only 1D cases are studied in this paper.

The method to compare the approximate techniques consists of two steps:

- In the first step, several narrow band methods are assessed against LBL calculations considering 1,000 rays emitted at several locations defined by the user inside the gaseous medium. These rays are statistically representative of the problem under study and comparisons of the results provided by the narrow band methods with LBL calculations allow choosing one of the narrow band models as a reference for calculations with a higher number of rays. The reference is not chosen arbitrarily, as is often the case [4], but determined through direct comparisons with LBL calculations.
- In the second step, when the reference model is chosen, calculations are performed for all models except LBL whose calculation cost in a deterministic spectral integration context is prohibitive. For this second step, a higher number of rays is selected (100,000 at each spatial location considered for the calculation). Comparisons of the various methods with the reference narrow band model yields a fair estimate of the accuracy of the various techniques in a true heat transfer context. This thus provides information relative to the applicability of a particular model to treat the case studied as well as estimates of its precision and computational cost.

The narrow band (449 narrow bands of 25 cm^{-1} width between 50 cm^{-1} and 11,250 cm^{-1}) and global methods considered in this work are described in the next sections. They are not detailed due to limited space, but references are provided where interested readers can find more information.

2.1 LBL and narrow band models

Line-By-Line (LBL) approach. This method is used as the reference for calculations with a small number of rays (1,000). This restriction is due to the computational time required by spectral integration at high resolution ($5x10^{-3}$ cm^{-1} for the LBL data used here). More details about these LBL datasets are available in Ref. [5]. The same LBL data are used to generate parameters for all methods.

Narrow band Ck models. Two narrow band Correlated / Comonotonic-*k* databases (with a number of gray gases equal to 4 or 7) were generated. The treatment of the gas mixture uses the double integration method [6]. Pseudo-spectral integration is performed using Gauss-Legendre quadratures restricted to the interval [0,1].

Narrow band ℓ-distributions. This method is applied with 1,000-point mapping functions [2]. It uses the Godson-Weinreb-Neuendorffer method [3] to handle path non-uniformities. This treatment of path non-uniformities is among the oldest (it was initially proposed in 1953 in a paper by Godson [7]) and also among the most accurate for treating non-uniform situations, as noticed by Young [3]. The method is applied without reordering of the paths since the gradients between two successive layers are small enough to avoid noticeable asymmetry issues. This problem of asymmetry was studied in depth in Refs. [8,9]. Transmissivities of gas mixtures are evaluated as the product of the transmissivities of the single species, providing a treatment of overlapping spectra that rigorously coincides with the one used for the narrow band C*k* methods.

2.2 Global methods of gas radiation

Weighted Sum-of-Gray-Gases. Under the assumptions of the WSGG model, the total emissivity of a uniform path of gas is given as:

$$\varepsilon\left(T, p_a L\right) = \sum_{j=1}^{J} a_j\left(T\right) \cdot \left[1 - \exp\left(-\kappa_{pj} \cdot p_a L\right)\right] \tag{1}$$

$$a_j\left(T\right) = \sum_{k=0}^{K} a_{j,k} \cdot T^k \tag{2}$$

where J is the number of gray gases (set to 4 in the present work), p_a the partial pressure of absorbing gas, T the gas temperature and L the length of the gas path.

Coefficients $a_{j,k}$ used to evaluate the gray-gases weights $a_j\left(T\right)$ are calculated for fixed mole fractions and are provided in Tables 1 (H_2O) and 2 (CO_2). They were calculated from the same detailed spectral database as all other methods [5]. They correspond to methane combustion in air at atmospheric pressure. A second set (condition of ethylene combustion in air, molar fraction of water vapor Y_{H_2O} = 0.13, and carbon dioxide Y_{CO_2} = 0.13) was also generated. This second set was not found to provide significant differences with those provided here when applied to our test cases. It is thus not reported here. Mixtures are treated by the double integration method. Application of the WSGG model within the frame of radiative heat transfer calculations in non-uniform media can be found in Ref. [10]. The method to obtain the WSGG coefficients is described in Ref. [11].

The Rank Correlated Spectral Line Weighted sum of gray gases (RC-SLW) method. The SLW method was initially described by Denison and Webb in Ref. [12]. RC-SLW is the most recent and advanced version of the SLW method, the main advantage of which is to avoid recourse to any reference state to make calculations in non-uniform media. This possible treatment of path non-uniformities within the frame of global methods was proven mathematically in Ref. [13]. The RC treatment can be applied to FSK methods, as shown in Ref. [14], and also to the ADF model [15]. Indeed, all these models are fundamentally the same theoretically, but the implementation of the methods (viz. the model including all possible treatments of LBL data to define model parameters) may be different, which is why they may sometimes provide distinct results. In the case of RC-SLW and RC-FSK, the two methods based on the same strategy to evaluate the weights are identical [14]. The RC-SLW model considered here uses extended ALBDF databases described in Ref. [16]. The treatment of gas

mixtures uses the multiplication approach [6]. RC-SLW model uses 16 gray gases. Reference source temperatures for the definition of weights are calculated as the volumetric average temperature of the gas, and are thus different in the three cases considered in this work. These cases are described in the next section.

Table 1: WSGG coefficients for H_2O at 1 atm with Y_{H_2O} = 0.2. Coefficients are valid for temperatures ranging from 300 to 3,000 K and path lengths from 0.001 to 30 m.

j	κ_{pj} (atm.m)$^{-1}$	$a_{j,0}$	$a_{j,1}$ (K^{-1})	$a_{j,2}$ (K^{-2})	$a_{j,3}$ (K^{-3})	$a_{j,4}$ (K^{-4})
1	0.24322	1.6411×10^{-1}	1.7180×10^{-4}	2.8874×10^{-8}	-3.3595×10^{-11}	4.2916×10^{-15}
2	1.6708	4.7244×10^{-2}	3.1740×10^{-4}	-1.5529×10^{-7}	9.0973×10^{-12}	3.0049×10^{-15}
3	8.9678	1.2590×10^{-2}	5.1559×10^{-4}	-5.6615×10^{-7}	2.1386×10^{-10}	-2.7534×10^{-14}
4	82.058	2.2156×10^{-1}	-3.4489×10^{-4}	2.1419×10^{-7}	-6.1766×10^{-11}	6.8412×10^{-15}

Table 2: WSGG coefficients for CO_2 at 1 atm with Y_{CO_2} = 0.1. Coefficients are valid for temperatures ranging from 300 to 3,000 K and path lengths from 0.001 to 30 m.

j	κ_{pj} (atm.m)$^{-1}$	$a_{j,0}$	$a_{j,1}$ (K^{-1})	$a_{j,2}$ (K^{-2})	$a_{j,3}$ (K^{-3})	$a_{j,4}$ (K^{-4})
1	0.45798281	2.4248×10^{-3}	3.7355×10^{-4}	-3.5321×10^{-7}	1.2474×10^{-10}	-1.5633×10^{-14}
2	4.58	7.0061×10^{-2}	-1.0403×10^{-4}	1.7807×10^{-7}	-9.2463×10^{-11}	1.4435×10^{-14}
3	44.2462062	7.5200×10^{-2}	-6.4676×10^{-5}	4.9758×10^{-8}	-2.2068×10^{-11}	3.4200×10^{-15}
4	397.54875	-9.7276×10^{-3}	1.3869×10^{-4}	-1.3644×10^{-7}	4.7644×10^{-11}	-5.7010×10^{-15}

2.3 Description of the test cases

All the test cases studied in this work consider hot gases at atmospheric pressure bounded by black walls. 1D geometries are treated. The temperature, in K, and species concentration profiles depend only on the distance from the left wall (located at x = 0). They follow the equations given below, where L is the distance between the walls.

Case C1: Sinusoidal temperature (in K) and species concentration profiles

$$T(x) = 700 - 300\cdot\cos(\pi x/L),\ Y_{H_2O}(x) = 0.2 - 0.15\cdot\cos(\pi x/L),\ Y_{CO_2}(x) = 2/3\ Y_{H_2O}(x) \quad (3)$$

with: L = 3 m.

Case C2: Hyperbolic temperature (in K) and species concentration profiles

$$T(x) = 1500 + 8000\cdot f(x),\ f(x) = (1/2 - x/L)^3,\ Y_{H_2O}(x) = 0.3 + 2.4\cdot f(x),\ Y_{CO_2}(x) = Y_{H_2O}(x)/2 \quad (4)$$

with: L = 2 m.

Case C3: Sinusoidal square temperature (in K) and species concentration profiles

$$T(x) = 500 + 2000\cdot\sin^2(\pi x/L),\ Y_{H_2O}(x) = 0.4\cdot\sin^2(\pi x/L),\ Y_{CO_2}(x) = Y_{H_2O}(x)/2 \quad (5)$$

with: L = 2 m.

For the radiative transfer calculations, the gas between the two walls was initially divided into 23 uniform layers. The corresponding temperature and composition of the gas were calculated at the center of these layers. A sensitivity analysis was performed to study the influence of this spatial discretization scheme on the results. Radiative powers and fluxes were found to be insensitive to the selection of a higher number of layers in cases C1 and C2. For case C3, the use of 69 layers was found to be necessary to obtain grid independence of radiative powers and fluxes.

3. RESULTS AND DISCUSSION

Results of comparisons of the various techniques are provided in Tables 3 to 5. Values of CPU times provided in the Tables are normalized by the CPU time for the WSGG model (which is 2 s for 1,000 rays / 200 s for 100,000 rays in cases C1-C2, i.e., 23 layers; 5.5 s / 555 s for case C3, i.e., 69 layers). Absolute errors (second column) is the mean absolute difference between the radiative powers calculated by the reference and the model listed in the first column; Rel. Error / max is the value of the absolute error (column 2) divided by the maximum radiative power given by the reference model.

In all the cases considered, the ℓ-distribution approach is found to provide results more accurate than both C*k*-4 and C*k*-7 when assessed against LBL calculations with 1,000 rays (first three lines in each table). Moreover, in terms of computational time, the ℓ-distribution approach is more efficient than C*k* models (a factor 2, in case C3, when compared to C*k*-4). The ℓ-distribution approach was thus chosen as the reference model for calculations with a higher number of rays, in all the 1D cases considered here.

Table 3: Case C1

Model	Absolute error (W/m^3)	Rel. Error / max (%)	Normalized CPU Time
1,000 Rays			
ℓ-distribution	39.59	0.35 %	129
Ck-7	139.04	1.23 %	488
Ck-4	301.59	2.67 %	205
100,000 Rays			
Ck-7	129.16	1.12 %	468
Ck-4	289.63	2.50 %	198
RC-SLW	308.00	2.66 %	64
WSGG	999.06	8.63 %	1

Table 4: Case C2

Model	Absolute error (W/m^3)	Rel. Error / max (%)	Normalized CPU Time
1,000 Rays			
ℓ-distribution	2963.31	0.61 %	131
Ck-7	4048.78	0.83 %	478
Ck-4	9146.08	1.88 %	206
100,000 Rays			
Ck-7	5860.38	1.29 %	477
Ck-4	10555.76	2.31 %	203
RC-SLW	10900.87	2.39 %	64
WSGG	36566.55	8.02 %	1

Table 5: Case C3

Model	Absolute error (W/m^3)	Rel. Error / max (%)	Normalized CPU Time
1,000 Rays			
ℓ-distribution	7564.16	0.61 %	96
Ck-7	10360.24	0.84 %	468
Ck-4	25165.25	2.04 %	201
100,000 Rays			
Ck-7	12721.11	1.05 %	458
Ck-4	24728.34	2.04 %	197
RC-SLW	30771.78	2.54 %	60
WSGG	26857.82	2.22 %	1

Profiles of radiative power are plotted in Figures 1 to 3 for 100,000 rays. At the top of the Figures, radiative powers calculated with the ℓ-distribution approach, chosen as the reference following the results with 1,000 rays provided in Tables 3-5, are given. At the bottom, absolute difference of several methods (C*k*-4, C*k*-7, WSGG and RC-SLW) w.r.t the ℓ-distribution solutions are shown.

The results provided in Tables 3-5 and Figures 1-3 show that:

- The ℓ-distribution approach provides the most accurate results in all 1,000 ray calculations, when compared with high resolution calculations, at a fraction of the cost of a LBL method (normalized CPU time for LBL is 71200-72300 for 1,000 rays for cases C1-2; 66909 for case C3). In all the configurations considered in the work, errors lower than 1% on radiative powers are observed with ℓ-distribution modelling.
- RC-SLW and C*k*-4 methods yield a similar accuracy. RC-SLW model is more CPU time consuming than WSGG, but the computation time can be drastically reduced by tabulating the model coefficients, i.e., the solutions of implicit equations. A tabulated version of RC-SLW model should theoretically yield a method as computationally efficient as WSGG.
- The WSGG method achieves a good accuracy, with errors lower than 10% in all the cases considered. This is quite remarkable, considering the simplicity of the method and its lack of dedicated treatment of path non-uniformities. In case C3, WSGG even provides more accurate results than RC-SLW, although this result cannot be considered as a general statement.
- Of all the methods studied in this work, the less convincing one is C*k*-7, which requires the highest computational cost (a factor of roughly 3.5 when compared to ℓ-distributions, 8 with RC-SLW), without improving the results significantly when compared to all other techniques.

Obviously, all these comments only apply to the set of problems considered here (black boundaries) and to the radiative solver used for the comparisons (stochastic ray tracing). The ℓ-distribution method, for instance, is formulated in terms of transmissivities: it cannot be applied, for now, with a discrete ordinate (DOM) solver of the RTE. On the other hand, all other models rely on a *k*-formulation: they can be applied with DOM. However, full spectrum techniques (RC-SLW and WSGG) are restricted, presently, to gray boundaries: ℓ-distribution and C*k* models are applicable to non-gray walls. These possible limitations of the methods need to be accounted for while choosing a specific approximate treatment of gas paths for engineering applications.

Finally, notice that in terms of memory space, the size of the database is 29,517 Mb for LBL dataset, 8,704 Mb for ℓ-distributions, 23 Mb and 90 Mb for C*k*-4 and C*k*-7 respectively and 23 Mb for RC-SLW. WSGG memory cost is negligible.

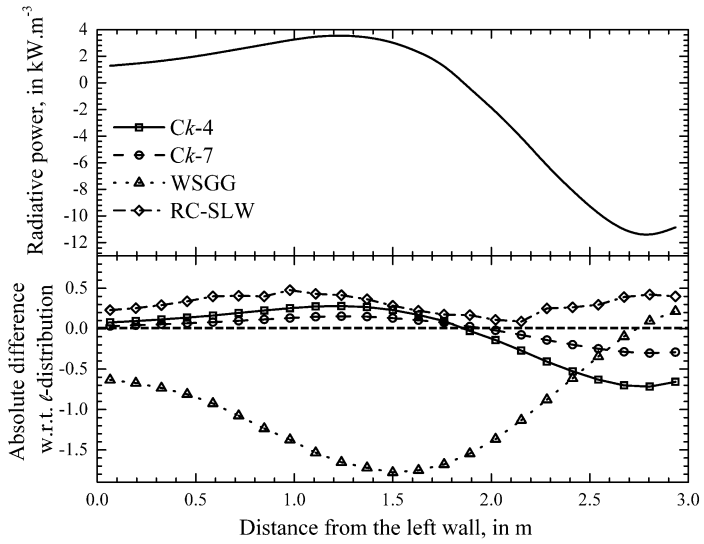

Figure 1. Case C1 (top: solid line – benchmark ℓ-distribution)

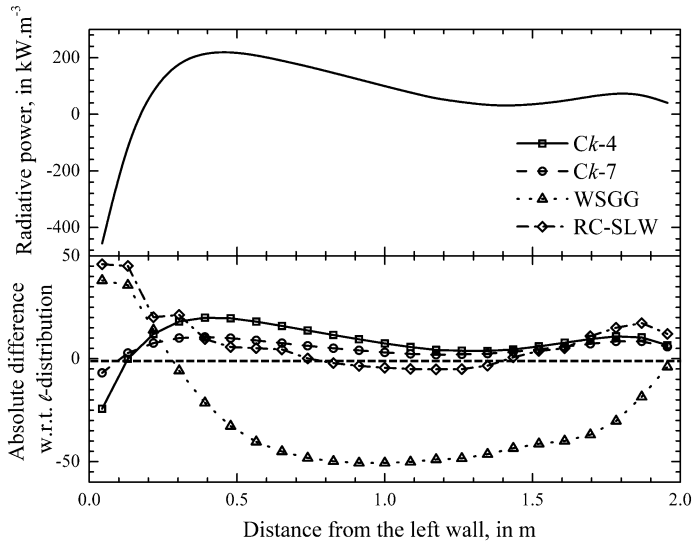

Figure 2. Case C2 (top: solid line – benchmark ℓ-distribution)

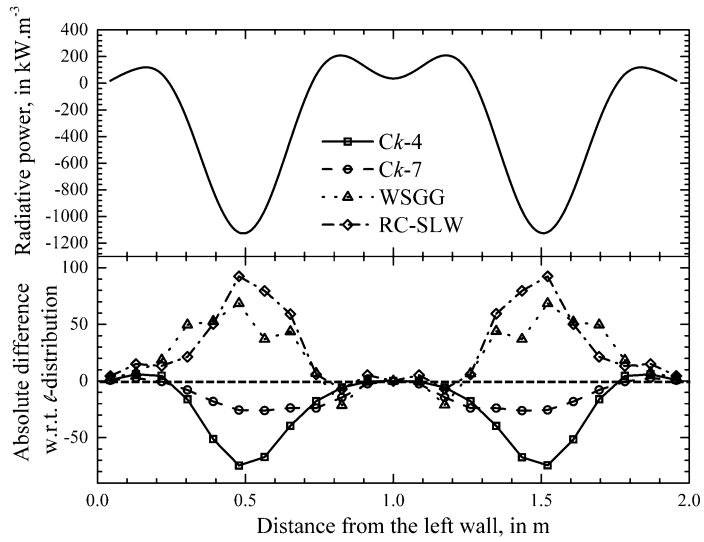

Figure 3. Case C3 (top: solid line – benchmark ℓ-distribution)

4. CONCLUSION

Many engineering problems involve complex interactions between fluid flows, chemical reactions, radiative heat transfer, etc. Each part of these multi-physics problems, considered separately, can now be simulated with a high accuracy: using Direct Numerical Simulation for fluid flows, full chemistry, line-by-line Monte Carlo calculations for gas radiation, Maxwell's equation solvers for scattering by particles, etc. However, despite the computer power available now, most coupled configuration studies still rely on approximate methods, such as Large Eddy Simulations for fluid flows. In the case of radiative transfer in gases, the approximate methods described and compared in the present paper were proved to deliver accurate estimates, and are sufficiently robust to be applied confidently in coupled situations. Results described in this work provide relevant estimates of the precision that one can expect in real engineering applications at high temperature.

REFERENCES

[1] V. P. Solovjov, F. André, D. Lemonnier, B. W. Webb, "The rank correlated SLW model of gas radiation in non-uniform media", *J. Quant. Spectr. Rad. Transfer*, vol. 197, pp. 26-44, 2017.

[2] F. André, "The ℓ-distribution method for modeling non-gray absorption in uniform and non-uniform gaseous media", *J. Quant. Spectr. Rad. Transfer*, vol. 179, pp. 19-32, 2016.

[3] S. J. Young, "Band model theory of radiation transport", The Aerospace Press, 2013 [ISBN: 978-1-884989-25-4].

[4] V. Goutière, F. Liu, A. Charrette, « An assessment of real-gas modelling in 2D enclosures », *J. Quant. Spectr. Rad. Transfer*, vol. 64, pp. 299-326, 2000.

[5] J. Pearson, "The development of updated and improved SLW model parameters and its application to comprehensive combustion prediction", PhD dissertation, Brigham Young University, Provo, UT, 2013.

[6] V. P. Solovjov, B. W. Webb, F. André, *Radiative Properties of Gases*, In: Kulacki F, editor. *Handbook of Thermal Science and Engineering*, New York, Springer, pp. 1-74, 2017.

[7] W. L. Godson, "Evaluation of infra-red radiative fluxes due to atmospheric water", *Quart. J. Roy. Met. Soc.*, vol. 79, pp. 367-379, 1953.

[8] F. André, "An analysis of symmetry issues in the ℓ-distribution method of gas radiation in non-uniform gaseous media", *J. Quant. Spectr. Rad. Transfer*, vol. 190, pp. 78-87, 2017.

[9] F. André, "Effective scaling factors in non-uniform gas radiation modeling", *J. Quant. Spectr. Rad. Transfer*, vol. 204, pp. 112-119, 2017.

[10] F. Cassol, R. Brittes, F. H. R. Franca, O. A. Ezekoye, "Application of the weighted-sum-of-gray-gases model for media composed of arbitrary concentrations of H_2O, CO_2 and soot", *Int. J. Heat Mass Transf.*, vol. 79, pp. 796-806, 2014.

[11] F. R. Coelho, F. H. R. Franca, "WSGG correlations based on HITEMP2010 for gas mixtures of H_2O and CO_2 in high total pressure conditions", *Int. J. Heat Mass Transf.*, vol. 127, pp. 105-114, 2018.

[12] M. K. Denison, B. W. Webb, "A spectral line based weighted-sum-of-gray-gases model for arbitrary RTE solvers", *ASME J. Heat Transfer*, vol. 115, pp. 1004-1012, 1993.

[13] F. André, V. P. Solovjov, D. Lemonnier, B. W. Webb, "Co-monotonic global spectral models of gas radiation in non-uniform media based on arbitrary probability measures: Theoretical foundations.", *J. Appl. Math. Modeling*, vol. 50, pp. 741-754, 2017.

[14] V. P. Solovjov, B. W. Webb, F. André, "The rank correlated FSK model for prediction of gas radiation in non-uniform media, and its relationship to the rank correlated SLW model", *J. Quant. Spectr. Rad. Transfer*, vol. 214, pp. 120-132, 2018.

[15] L. Pierrot, Ph. Rivière, A. Soufiani, J. Taine, "A fictitious-gas-based absorption distribution function global model for radiative transfer in hot gases", *J. Quant. Spectr. Rad. Transfer*, vol. 62, pp. 609-624, 1999.

[16] B. W. Webb, V. P. Solovjov, F. André, "An exploration of the influence of spectral model parameters on the accuracy of the rank correlated SLW model", *J. Quant. Spectr. Rad. Transfer*, vol. 218, pp. 161-170, 2018.