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New H_2O weighted sum of gray gases model for natural convection flows within large cavities

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Abstract. Radiation heat transfer plays a significant role in buoyancy driven flows for large scale facilities. In the analysis of nuclear containment safety during severe accidents, it has been found that the thermal radiation particularly affects the temperature distribution and containment pressurization due to the humidity environment. In order to model thermal radiation, one of the main challenges is the description of nongray gas property for the steam-air mixtures. The weighted sum of gray gases model (WSGG) is a reasonable method in engineering applications because of its computational efficiency. There are many WSGG models available for combustion applications, but none of them is dedicated for low temperature applications. Furthermore, most of the existing WSGG models only provide the fixed partial pressure ratios (e.g., $p_{H_2O} = 2p_{CO_2}$ for methane). To overcome this limitation, a tailored WSGG model is derived by the Line-by-Line model for a gas mixture composed of arbitrary concentrations of H_2O. This tailored WSGG model is valid for the pressure path length ranging from 0.0001 to 10 $atm \cdot m$, and for the temperature from 300 to 1200 K. The WSGG correlations are verified against the Line-by-Line benchmark solutions with isothermal/non-isothermal temperatures and homogeneous/non-homogeneous concentrations. The results demonstrate the ability and efficiency of the new tailored WSGG formulation.

1. Introduction

During a severe accident in nuclear power plants, amounts of steam and hydrogen are released into the reactor containment building (e.g. 70,000 m^3 for German 1300 MW_e PWR). The stratification of hydrogen is located at the top of the containment building, and it is the main consideration of containment safety. The containment building is the last line of defense to avoid radioactive materials into the atmosphere and challenged by the hydrogen explosion. Hence, the prediction of hydrogen gas distribution during a severe nuclear accident is important for implementing effective hydrogen mitigation methods to ensure the integrity of containment buildings. The CFD computation as a tool to assess hydrogen transport and gas mixing processes in a reactor containment is increasingly applied in the recent past.

In the previous time, thermal radiation phenomenon was neglected in low temperature applications ($\leq 800\,K$) within large cavities. But recently, many experiments have shown that thermal radiation, even at low temperature levels and small gradients, may play a significant role in natural convection flows within large cavities. Experiments at the small scale facility DIANA [1] and the large scale facility PANDA [2] (PSI, Switzerland) have been performed to understand the interaction between natural convection, buoyancy turbulence and thermal radiation. Besides the surface net radiation, the different concentrations of steam-helium-air mixtures are taken into account to investigate the stratified layer erosion. In those applications, the nongray gas radiation cannot be neglected to predict the gas mixing process. It is concluded that the nongray gas model affects the radiation source term in the energy equation, since the radiative heat transfer may be of the same order as the convective heat transfer [3].

However, the description of nongray gas property is still a difficult task, even for steam vapor mixtures. For CFD engineering calculations, the WSGG model is a computation reasonable method for radiative heat transfer analysis. The WSGG model concept was first presented by Hottel and Sarofim [6], in which the whole spectrum is represented by a few gray gases with the specific temperature weighting factor. The WSGG model assumes the absorption coefficient is not dependent on the media temperature, but the weighting factors are temperature dependent. Unfortunately, most of the nongray gas models are developed for combustion applications, but not for low temperature applications. The another limitation of the WSGG model is the fixed molar ratios for the specific combustion, not arbitrary concentrations in real applications. To overcome this limitation, Cassol et al. [8] proposed a new approach for arbitrary concentrations of H_2O, CO_2 and soot for the combustion. However, the temperature range is far from the containment applications.

Therefore, the aim of this paper is to develop a tailored WSGG model for low temperature applications based on the HITRAN2016 [10] database. This paper is scheduled as follow. The Line-by-Line model is briefly introduced in Section 2, which is the most accurate model. The next Section 3 is focused on the WSGG coefficient algorithm, in which how to generate the tailored WSGG correlations is described. After that, the one-dimensional test cases for isothermal/non-isothermal and homogeneous/non-homogeneous are discussed.

2. Line-by-Line model

The spectral absorption coefficient is a complex function, which depends on the local temperature, total pressure, and partial pressure [5]. In this paper, the Lorentz profile [11] is chosen to obtain the spectral absorption coefficient

$$\kappa_\eta = N(p,T)Y \sum_i \frac{S_i(T)}{\pi} \frac{\gamma_i}{\gamma_i^2 + (\eta - \eta_i)^2} \tag{1}$$

where $N(p_s, T)$ is the number of gas molecules; p_s is the specie partial pressure; $S_i(T)$ is the line intensity of line i; η_i is the line location; γ_i is the line half-width; T is the media temperature. The half-width γ_i for the i-th line can be computed from HITRAN2016 database.

$$\gamma_i = \left(\frac{T_{ref}}{T}\right)^{n_{air}} [p_s \gamma_{s,i} + (p - p_s)\gamma_{air,i}] \tag{2}$$

where n_{air} is the coefficient of the temperature dependence of the air-broadened half width; γ_s is the self broadening half width; γ_{air} is the air broadening half width. Those parameters are provided in HITRAN database at the reference temperature 296 K. From the HITRAN2016 database, the self-broadening width for steam is greater than for carbon dioxide. This is the reason why the steam absorption coefficient is more complex than CO_2.

After obtaining the absorption coefficient, the reference Line-by-Line emissivity can be expressed as

$$\epsilon_{LBL} = \frac{\int_{\eta=0}^{\infty} I_{b\eta}(T)\,[1 - exp(-\kappa_\eta L)]\,d\eta}{\sigma T^4/\pi} \tag{3}$$

The HITRAN Application Programming Interface (HAPI) [7], which is written in Python, is published by the Harvard-Smithsonian Center for the remote access and the Line-by-Line spectral calculation. In this paper, the spectral discretization is set at $\Delta\eta = 0.01\ cm^{-1}$ to calculate the spectral absorption coefficient.

3. WSGG model

The WSGG model was proposed by Smith et al. [13], in which the whole spectrum is represented by a few gray gases with the specific temperature weighting factor. The total emissivity of a nongray gas media for a path length L is given as

$$\epsilon = \sum_{i=1}^{N} a_i(T)[1 - exp(-\kappa_i pL)] \tag{4}$$

$$a_i(T) = \sum_{j=0}^{N} b_{i,j} T^j \tag{5}$$

where N is the number of gray gases; p_s is the partial pressure; $a_i(T)$ is the weight for gray gas κ_i; $b_{i,j}$ is the temperature weighting coefficient. Normally the number of gray gases N equals to 3 or 4. In additional to the gray gases, there is a transparent gas for $i = 0$ ($\kappa_0 = 0\, m^{-1}$). The transparent gas weight is calculated by $1 - \sum_{i=1}^{N} a_i(T)$.

One of the main challenges is the description of the nongray gas property for different concentrations of steam-air mixture for high humidity applications. In order to determine the WSGG coefficients, the coefficient optimization fitting problem based on the total emissivity is shown in Eq. (6) [9][13]. In this paper, the number of nongray gases is 4.

$$\begin{aligned} \min \quad & \sum_{k=1}^{N_L \cdot N_T \cdot N_p} (\epsilon_{LBL} - \epsilon_{WSGG})^2 \\ \text{s.t.} \quad & 0 < a_i(T) < 1 \;\; (i = 0,1,2,3,4) \\ & a_i(T) = \sum_{j=0}^{4} b_{i,j} T^j \;\; (j = 0,1,2,3,4) \\ & a_0 = 1 - \sum_{i=1}^{4} a_i(T) \end{aligned} \tag{6}$$

where N_T is the number of temperature points; N_L is the number of beam length points; N_p is the number of steam partial pressure points, ϵ_{LBL} is the total emissivity calculated from the Line-by-Line model; ϵ_{WSGG} is the total emissivity calculated from the new tailored WSGG model.

For steam-air mixtures, an emissivity database is generated using the Line-by-Line model for $N_L = 44$ beam length points from 0.01 to 10 m, $N_T = 15$ temperature points from 300 to 1200 K with the uniform interval, and $N_p = 5$ steam partial pressures at 0.01, 0.1, 0.2, 0.4 and 1 atm. Hence, a total of 44*15*5 = 3300 emissivities are computed by the Line-by-Line model.

Actually this is a nonlinear optimization problem. The nonlinear optimization solvers exploit the Newton iteration to minimize the objective function, in which the gradient is compulsory. However, the objective function gradient oscillates rapidly by the reason of exponential function and fourth power of temperature. Yin et al. [4] proposed a modified WSGG model by giving the reference temperature 1200 K. But it is dedicated for combustion applications. In this paper the optimization problem is divided into two steps. The first step is to determine the band absorption coefficient κ_j. The band absorption coefficient is generated from the HITRAN2016 database, diving the whole spectrum into four bands (0-1000 cm^{-1}, 1000-2000 cm^{-1}, 3500-4000

Table 1: WSGG coefficients for H_2O with four gray gases

j	$\kappa_{p,j}$ $(atm \cdot m)^{-1}$	$b_{j,0}$	$b_{j,1}(K^{-1})$	$b_{j,2}(K^{-2})$	$b_{j,3}(K^{-3})$	$b_{j,4}(K^{-4})$
1	0.247	2.36676088×10^{0}	-1.48861386×10^{-2}	3.54432832×10^{-5}	-3.39746119×10^{-8}	1.14336477×10^{-11}
2	2.092	-1.60030849×10^{0}	1.07577415×10^{-2}	-2.33051655×10^{-5}	2.15168099×10^{-8}	$-7.14015090\times10^{-12}$
3	8.231	-1.32395362×10^{-1}	1.23327839×10^{-3}	-2.15773994×10^{-6}	1.63499215×10^{-9}	$-4.57726377\times10^{-13}$
4	64.321	3.57653399×10^{-1}	-1.48485499×10^{-3}	3.10297221×10^{-6}	-2.89422398×10^{-9}	9.67128899×10^{-13}

Valide for temperatures between 300 K and 1200 K and 0.0001 atm m $\leq$ ps $\leq$ 10 atm m.

cm^{-1} and the rest part). And the average absorption coefficient is calculated for each band. Those absorption coefficients are the initial guess for the WSGG model. If the absorption coefficients are determined, this equation becomes a linear equation. It is easy to apply the least square method to get $b_{i,j}$, shown in Eq. (7). If the numerical error is too large, the gradient descent method is applied to obtain better estimation.

$$\begin{bmatrix} (1-e^{-\kappa_1 pL}) & (1-e^{-\kappa_1 pL})T_1 & . & . & . & (1-e^{-\kappa_4 pL})T_1^4 \\ (1-e^{-\kappa_1 pL}) & (1-e^{-\kappa_1 pL})T_2 & . & . & . & (1-e^{-\kappa_4 pL})T_2^4 \\ . & . & & & & . \\ . & . & & & & . \\ . & . & & & & . \\ (1-e^{-\kappa_1 pL}) & (1-e^{-\kappa_1 pL})T_N & . & . & . & (1-e^{-\kappa_4 pL})T_N^4 \end{bmatrix} \begin{bmatrix} b_{1,0} \\ b_{1,1} \\ . \\ . \\ . \\ b_{4,4} \end{bmatrix} = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ . \\ . \\ . \\ \epsilon_N \end{bmatrix} \tag{7}$$

$$Ab = \epsilon \implies A^{tr}Ab = A^{tr}\epsilon \implies b = (A^{tr}A)^{-1}A^{tr}\epsilon \tag{8}$$

Figure 1 and Figure 2 compare the emissivities obtained from the Line-by-Line model, the new tailored WSGG model and the Cassol et al. [8] model, at four length-lengths: 0.01, 0.1, 1.0, and 10 m. Both cases are at the atmospheric environment with the remaining transparent nitrogen gas. The only difference between Figure 1 and Figure 2 is the steam pressures (0.2 and 0.8 atm). Globally both WSGG models are analogous to the Line-by-Line model. However, the tailored WSGG model provides improved values in the temperature range below 1000 K. Obviously the new steam WSGG correlatons is suitable for high steam concentrations in low temperature environment.

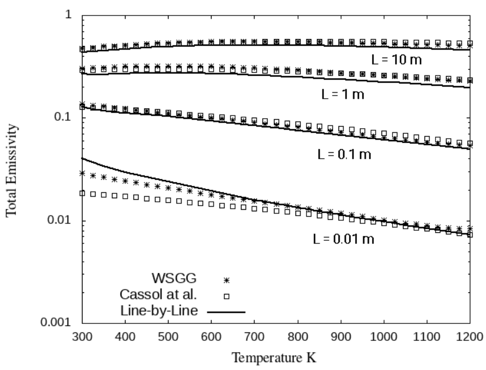


Figure 1: Comparison of the total emissivity from Line-by-Line integration model(p_{H_2O}=0.2)

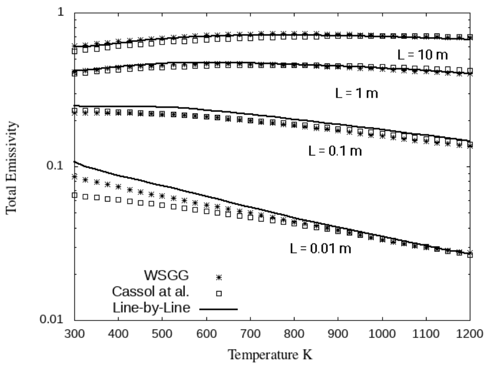


Figure 2: Comparison of the total emissivity from Line-by-Line integration model(p_{H_2O}=0.8)

4. Results and verification

4.1. one-dimensional slab cases

The simplest one-dimensional test cases proposed by Kim et al. [12] are chosen to verify the new tailored WSGG coefficients. This test case is a one-dimensional slab with two infinite plates at $X = 1.0$ meter distance, setting 100 uniform grids. The left and right plates are kept 0 K with the black wall. Both cases are at atmospheric conditions with the remaining transparent nitrogen gas. As shown in Table 2, the H_2O molar fraction and temperature are the function of the distance x.

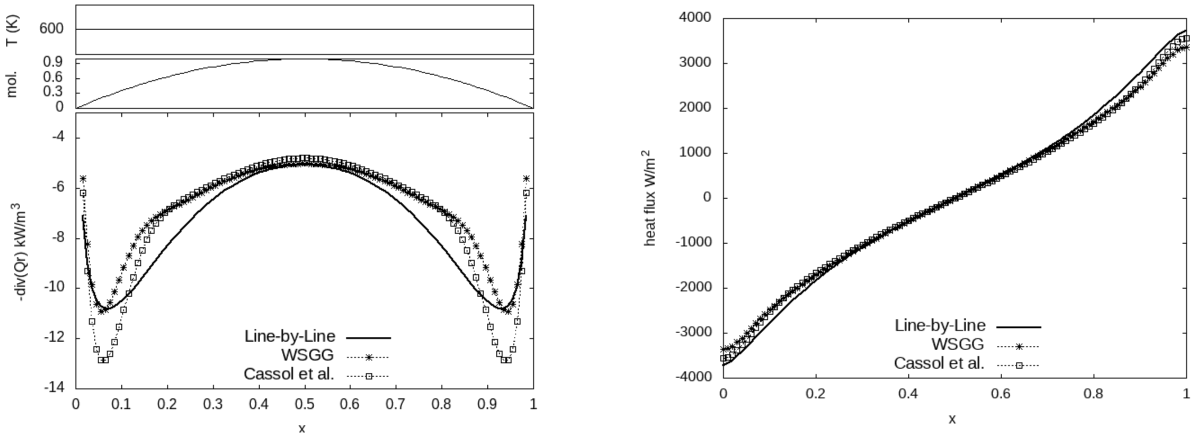
Table 2: 1D verification cases

Case	Participating gas	Temperature (K)	Concentration (vol%)
1	H_2O	Isothermal: 600 K	Non-homogeneous Eq. (9)
2	H_2O	Non-isothermal: Eq. (10)	Non-homogeneous Eq. (10)

$$c_{steam}(x) = 4(1-x)x \tag{9}$$

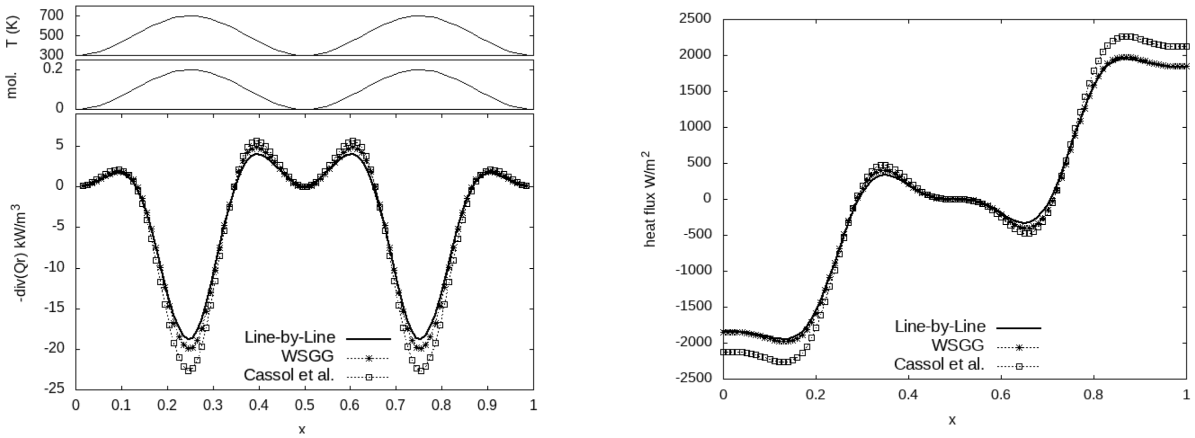
$$\begin{aligned} T(x) &= 300 + 400 sin^2\left(2\pi x\right) \\ c_{steam}(x) &= 0.2\, sin^2\left(2\pi x\right) \end{aligned} \tag{10}$$

The radiative heat source term and wall heat flux for test case 1 are shown in Figure 3. For the radiative source term, there is a steep slope near the cold walls, and the maximum radiative source term is found at the regions near 0.1 m. This is due to the low steam concentration near the walls even though this is a homogeneous temperature test case. From the Eq. (9), there is a steep increase for the steam concentration from 0 to 0.1 m. The cells near $x = 0.1$ m emits more energy into the cold wall than the absorption energy from the center of the domain. In the center, two WSGG models predict the radiative source in a good agreement with the Line-by-Line integration. However, the Cassol et al. WSGG model overpredicts the radiative source term at $x = 0.1$ m. Globally the average error for the new tailored WSGG is 6.70 % in comparison with the Line-by-Line model; while 10.20 % for the Cassol et al. WSGG model.
The radiative heat source term and wall heat flux for test case 2 are shown in Figure 4. The radiative source term near the wall is positive in this case, which means the absorption of energy is larger than its emission energy. In principle, the radiative energy balance not only relies on the nearest cells but also the local region because of gas transmissivity. The maximum radiative emission point is near $x = 0.25$ m, with the highest concentration and temperature. In the



(a) radiative source term (b) wall heat flux

Figure 3: Radiation source term and wall heat flux for case 1



(a) radiative source term (b) wall heat flux

Figure 4: Radiation source term and wall heat flux for case 2

center, the radiative source term becomes around zero again owing to the lowest temperature at this point. For the radiation heat flux at $x < 0.2$ m region, there is a significant difference between the the tailored WSGG model and the Cassol et al. WSGG model. The maximum relative error for the new tailored WSGG and the Cassol et al. WSGG are 5.91 % and 20.13 %, respectively.

5. Conclusion and Future Work

This paper presents a new algorithm to determine the WSGG coefficients by utilizing the high-resolution spectral HITRAN2016 database for low temperature applications. Firstly, a Line-by-Line emissivity database for different temperatures, pressures and path-lengths is generated by the HITRAN2016 HAPI. For the WSGG coefficients fitting problem, it is divided into two steps. The non-temperature dependent gray gas absorption coefficients are determined from the HITRAN2016 database. Then, the least squares method is used to obtain the temperature-dependent weighting coefficients. For the second part of this paper, this tailored WSGG model is verified against the Line-by-Line model for the one-dimensional cases. There is a visible accuracy improvement for the new tailored WSGG model in comparison with other WSGG models at low temperature/high steam conditions.

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