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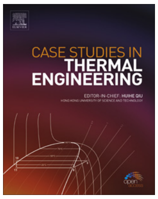

Accuracy evaluation of the gray gas radiation model in CFD simulation

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ABSTRACT

Gaseous combustion product, a mixture of radiating gas CO_2, H_2O and nonradiating gas N_2, O_2, absorbs and emits radiation spectrally selectively. Accurate simulation of radiation heat transfer inside a combustion chamber requires the line-by-line radiation model which is impossible for engineering practice because of the prohibitive computation time cost. The simplified gray gas model is the most popular model used in engineering CFD simulation. However, the accuracy of this model has not been systematically evaluated. Several radiation heat transfer cases have been simulated with the gray gas model and the simulation accuracy has been evaluated by the simulation result with the more accurate Statistical Narrow Band model. It is shown that the CFD simulation with the gray gas model can predict the peak heat transfer flux location accurately, but will over predict the heat flux and the heat transfer rate by as much as 23% for the tested cases.

1. Introduction

Inside a combustion chamber, both convection and radiation heat transfer exist. Since the temperature of gaseous combustion product is high, radiation heat transfer is strong and it is the dominant heat transfer mechanism for large and slow flow combustion devices such as gas furnaces. The accurate calculation of radiation heat transfer inside combustion chamber is crucial for the prevention of local overheating and the overall energy balance of combustion chamber. CFD software solves the radiation transfer equation to resolve the radiation heat transfer between gas and combustion chamber wall. The radiation absorption coefficient k_λ (unit of m^{-1}) is an input parameter for the radiation transfer equation. The radiation absorption coefficient is a function of wavelength, gas composition, pressure, and temperature.

Combustion product is a mixture of radiating gases CO_2 and H_2O and nonradiating gases N_2 and O_2. The polar gas molecules (CO_2 and H_2O) emit or absorb thermal radiation when the internal energy level transition occurs. Their radiation spectrum are a large number of discrete spectral lines broadened by collision broadening and Doppler broadening. The exact description of these broadened spectral lines is called the line-by-line model [1]. To use the line-by-line model, each band has to be divided into thousands of wavelength or wavenumber (inverse of wavelength) intervals and each interval has an individual value of absorption coefficient. The whole spectrum would result in hundreds of thousands wavelength intervals and the radiation transfer equation needs to be solved for each wavelength interval in the whole flow field; this results in prohibitive computation cost. Approximations and simplifications have to be adopted in engineering CFD simulation for

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thermal radiation in combustion chambers. Depending on whether the approximate absorption coefficient depends on wavelength or not, simplified models can be divided into the Statistical Narrow Band (SNB) model, wide band model, and gray gas model [1]. For all of them, the radiation absorption coefficient is a function of gas composition, temperature, pressure, and the characteristic length of combustion chamber now. In contrast, the absorption coefficient of the line-by-line model is a physical property of the gas which is independent of combustion chamber size. The gray gas model assumes that the gas is gray and it uses an average absorption coefficient over the whole spectrum. The narrow band and wide band models divide the spectrum to different numbers of spectral bands and adopt different absorption coefficients for the bands.

In present study, the methods of the gray gas model and the SNB model were briefly introduced first; they were used in the simulation of several test cases. Then, the accuracy of the gray gas model is evaluated with the more accurate SNB simulation result.

2. Manual calculation with the gray gas model

The gray gas method was proposed by Hottel [2,3] and is used to determine the incident radiation heat flux from H_2O or CO_2 with temperature T_g on combustion chamber wall.

$$E_g = \varepsilon_g \sigma T_g^4 \tag{1}$$

The gas emissivity ε_g is a function of temperature, gas composition, pressure, and the characteristic length of combustion chamber L. For any location on the wall, L_{local} is the solid angle weighted average length of all incident radiation beams from the boundary of gas volume. L is the average value of L_{local} of all element wall surface representing the mean radiation beam length of combustion chamber. L can be approximately calculated with [3]

$$L = 3.6V/A \tag{2}$$

V and A are the volume and the surface area of combustion chamber respectively. For the mixture of H_2O or CO_2 and nonradiating gas at 1 atm static pressure, the gas mixture emissivity ε_g can be obtained from Hottel chart [3]; the emissivity data is experimental data or experimental data extrapolated. For the mixture of H_2O and CO_2 and nonradiating gas at different static pressure p, the mixture emissivity ε_g can be calculated as

$$\varepsilon_g = C_{H_2O}(p, p_{H_2O}, L)\varepsilon_{H_2O}(T_g, p_{H_2O}L) + C_{CO_2}(p, p_{CO_2}, L)\varepsilon_{CO_2}(T_g, p_{CO_2}L) - \Delta\varepsilon(T_g, p_{H_2O}, p_{CO_2}, L) \tag{3}$$

where C_{H_2O} and C_{CO_2} are the pressure correction factors for H_2O and CO_2 in a mixture with static pressure p deviating from 1 atm respectively, ε_{H_2O} and ε_{CO_2} are the component emissivity for H_2O and CO_2 with partial pressure p_{H_2O} and p_{CO_2} respectively. $\Delta\varepsilon$ is the mixture correction factor accounting for the spectrum overlap of H_2O and CO_2. All these parameters can be obtained from Hottel charts [3]. Unfortunately, all the data in Hottel chart was from his experimental data in 1954, the experimental uncertainty of the data is huge; especially, the data for high temperature gas was just the extrapolation of the low temperature experimental data, the error is tremendously large. Leckner [4] provided more accurate data for a wide range of temperature; his data is used for the following simulations.

The incident radiation rate on combustion chamber wall q_e can be calculated as

$$q_e = AE_g = A\varepsilon_g \sigma T_g^4 \tag{4}$$

If combustion chamber wall surface is blackbody, this incident radiation rate will be completely absorbed. Combustion chamber wall emits thermal radiation (continuous spectrum) too; the radiation from the solid wall will be partially absorbed by the gas spectrally selectively when it passes through the gas. The radiation from combustion chamber wall will be absorbed by combustion product with the rate [3]:

$$q_a = A\alpha_g \sigma T_s^4 \tag{5}$$

$$\alpha_g = \alpha_{H_2O} + \alpha_{CO_2} - \Delta\alpha \tag{6}$$

$$\alpha_{H_2O} = (T_g/T_s)^{0.45} C_{H_2O}(p, p_{H_2O}, L)\varepsilon_{H_2O}(T_s, p_{H_2O}LT_s/T_g) \tag{7}$$

$$\alpha_{CO_2} = (T_g/T_s)^{0.65} C_{CO_2}(p, p_{CO_2}, L)\varepsilon_{CO_2}(T_s, p_{CO_2}LT_s/T_g) \tag{8}$$

$$\Delta\alpha = \Delta\varepsilon(T_s, p_{CO_2}, p_{H_2O}, T_sL/T_g) \tag{9}$$

α_g is the absorsivity of the mixture to the incident radiation from the blackbody wall with temperature T_s. The net radiation heat transfer rate between the gas and the blackbody chamber wall:

$$q_{net} = A\sigma(\varepsilon_g T_g^4 - \alpha_g T_s^4) \tag{10}$$

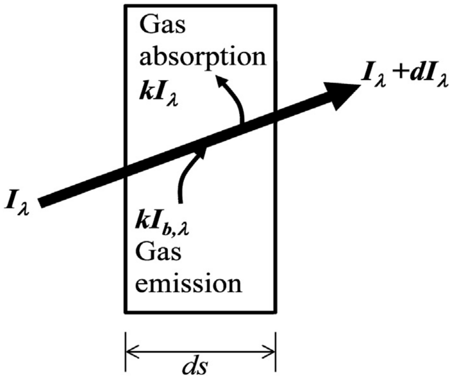

Fig. 1. Schematic of the volumetric emission and absorption of gas radiation.

The radiation heat transfer rate between gas mixture and blackbody wall can be calculated with Eqs. (2)–(10) and the charts in Leckner [4]. The local heat transfer flux at some location of chamber wall could be calculated with Eq. (1), Eq. (3) and L_{local}. However, L_{local} is not easy to be obtained since it is a solid angle weighted average radiation beam length. Even for the chamber with simple geometry such as a hemisphere, only L_{local} at the center of the base plane can be obtained easily: it is the radius of the sphere. L_{local} at other locations of the spherical surface and the base plane could be judged qualitatively but is hard to be evaluated quantitatively. Manual calculation with the gray gas model is eligible for the total heat transfer rate calculation between combustion product and blackbody wall.

3. CFD simulation with the gray gas model

In engineering practice, engineers are not only interested in the total heat transfer rate but also the heat flux distribution, especially the maximum heat flux value and its location. The manual calculation method introduced by Hottel obviously does not give out all the desired information. Heat flux distribution can be obtained by solving the radiation transfer equation with CFD software. For the situation without scattering, the radiation transfer equation is (Fig. 1)

$$\frac{dI_\lambda}{ds} + k_\lambda I_\lambda = k_\lambda I_{b,\lambda} \tag{11}$$

where I is the radiation intensity, s is the length of radiation path, λ is the wavelength, $I_{b,\lambda}$ is the radiation intensity of blackbody, and k_λ is the spectral absorption coefficient. The second term on the left represents the absorption of incident radiation by gas and the term on the right represents the gas emission (spectral absorption coefficient = spectral emission coefficient). The radiation transfer equation is discretized in space and solved numerically to get the radiation intensity in different directions of all mesh cells. The line-by-line model gives the accurate value of spectrally dependent absorption coefficient, but using this accurate model is prohibitive as explained before. An appropriate spectrally independent average absorption coefficient is needed for the gray gas model in CFD simulation. The following equation can be used to calculate it.

$$k = -\ln(1-\varepsilon_g)/L \tag{12}$$

Emissivity ε_g and characteristic length L are obtained from the gray gas model in Section 1. The chart data was fitted to equations and a user subroutine was coded with the fitted equations. During CFD simulation, the subroutine calculates the local emissivity according to the local temperature, pressure, gas composition, and the global characteristic length L, then the local absorption coefficient is calculated with Eq. (12). This is the popular gas radiation simulation method in the CFD simulation for industrial furnaces.

4. CFD simulation with the SNB model

The narrow band model divides the spectrum to hundreds of narrow bands, each band interval has its own absorption coefficient which is often obtained experimentally representing the overall radiation effect of the band. This model is not equivalent to the accurate line-by-line model. It is the result of a statistical assumption of band structure, the parameters of the statistical model were obtained by fitting the experimental band emissivity. This model can predict radiation heat transfer with spectral dependence and is much more accurate than the gray gas model. However, the computation cost is still very high since the radiation transfer equation has to be solved several hundred times in the whole flow field.

CFD simulation with the narrow band model is to solve the radiation transfer equation for every spectral band and the band absorption coefficient can be calculated with the method introduced in NASA reports [5,6].

$$k_i = k_{i,0}\frac{p_{\mathrm{H_2OorCO_2}}T_0}{p_0 T} \Big/ \sqrt{1 + k_{i,0}\frac{p_{\mathrm{H_2O\ or\ CO_2}}T_0}{p_0 T}\frac{L}{4a_i}} \tag{13}$$

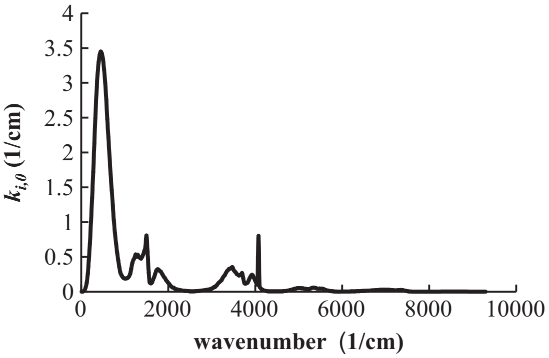

Fig. 2. Spectral absorption coefficient of water vapor at 2000 K and 1 atm.

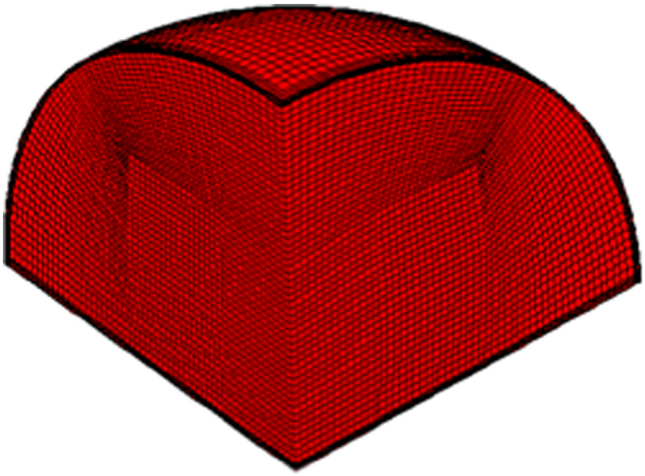

Fig. 3. The mesh.

$$a_i = \gamma / d_i \tag{14}$$

$$H_2O:\ \gamma = 0.09p\sqrt{T_0/T} + 0.44p_{H_2O}T_0/T \tag{15}$$

$$CO_2:\ \gamma = 0.07p\sqrt{T_0/T}(1+0.28p_{CO_2}/p) \tag{16}$$

where $k_{i,0}$ is the spectral absorption coefficient of the ith band reduced to the standard condition (T_0=273 K, p_0=1 bar), k_i is the absorption coefficient at the operating condition (p, T), a_i is the line density of the ith band, d_i is the average line spacing of the ith band, γ is the average half width of the spectral lines of the ith band. The radiation absorption coefficient of gas mixture is equal to the sum of the absorption coefficients of H_2O and CO_2.

$k_{i,0}$ and d_i at different temperatures can be found in NASA reports [5,6]. The radiation spectrum spans wavenumber 50–9300 cm^{-1} and there are total 370 bands with bandwidth 25 cm^{-1}. Fig. 2 shows an example of the band absorption coefficient of H_2O reduced to the standard condition.

The simulations with both the gray gas model and the SNB model in the following section are carried out with the Star-CCM software.

5. Simulation examples

Case 1. The radiation heat transfer within a hemisphere with 2.5 m radius. The hemisphere is full of 2000 K, 1 atm water vapor; the spherical surface and the base plane surface is blackbody with 0 K temperature. Only $\frac{1}{4}$ of the geometry is simulated because of symmetry (Fig. 3). The S8 discrete ordinate method (the 4π solid angle of each cell is discretized evenly to 80 pieces, each piece of solid angle has its own radiation intensity) is used for spatial discretization of the radiation transfer equation.

Manual calculation with the gray gas model in Section 1: L=2 m, ε_g=0.4323, total heat transfer rate to the wall=23.1 MW.

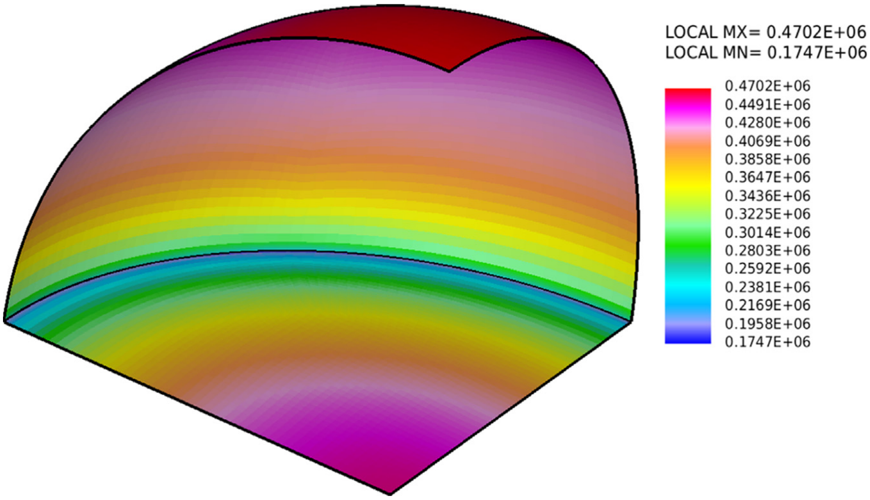

Fig. 4. The incident radiation heat flux on the wall of the CFD simulation result with the gray gas model for case 1.

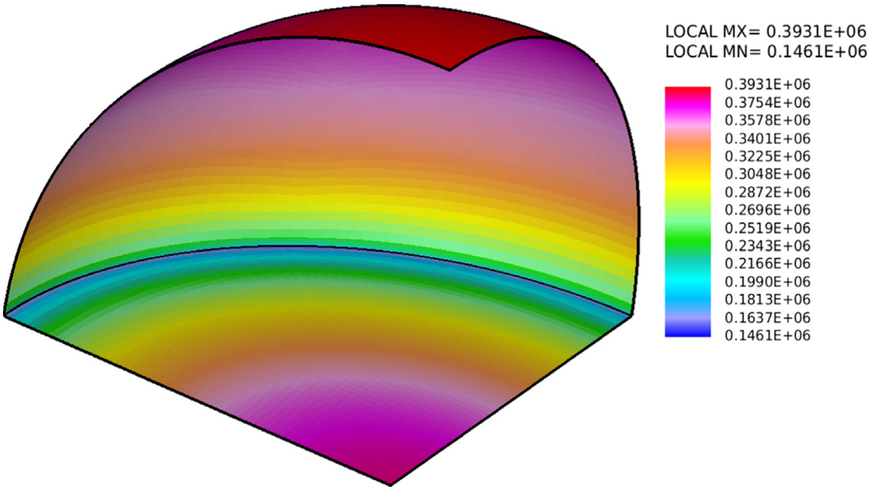

Fig. 5. The radiation heat transfer flux on the wall of the CFD simulation result with the gray gas model for case 2.

CFD simulation with the gray gas model in Section 2: $k=0.2831\ \text{m}^{-1}$ (resulted from $L=2$ m, $\varepsilon_g=0.4323$), total heat transfer rate to the wall = 23.4 MW.

Since the absorption coefficient of the CFD simulation came from the gray gas model, it is no wonder that the total heat transfer rate of the two methods are very close (1.2% difference). The main difference between them is that the manual calculation assumes an uniform distribution of radiation heat flux while the CFD simulation considers the variation of heat flux on the wall.

Fig. 4 shows the incident radiation flux on the solid wall. Its peak value is located on the top of the spherical surface with the value 0.47 MW/m^2; the minimum value is 0.175 MW/m^2 and located at the edge connecting the spherical surface and the base plane surface. The value at the base surface center is 0.457 MW/m^2, the corresponding manually calculated value with $L_{local}=2.5$ m (the exact local beam length) is 0.424 MW/m^2 (this value should be considered as the accurate one) which is 7.2% lower than the CFD result.

Case 2. Everything is the same as in case 1 except that the wall temperature is 1273 K now.

Manual calculation with the gray gas model in Section 1: $L=2$ m, $\varepsilon_g=0.4323$, $\alpha_g=0.5658$, net heat transfer rate to the wall = 18.14 MW.

CFD simulation with the gray gas model in Section 2: $k=0.2831\ \text{m}^{-1}$ (resulted from $L=2$ m, $\varepsilon_g=0.4323$), net heat transfer rate to the wall = 19.54 MW, maximum heat flux = 0.3931 MW/m^2, minimum heat flux = 0.1461 MW/m^2, heat flux at the base center = 0.3818 MW/m^2 (Fig. 5).

CFD simulation with the SNB model in Section 3: net heat transfer rate to the wall = 18.1332 MW, maximum heat flux = 0.3507 MW/m^2, minimum heat flux = 0.1393 MW/m^2, heat flux at the base center = 0.3481 MW/m^2 (Fig. 6).

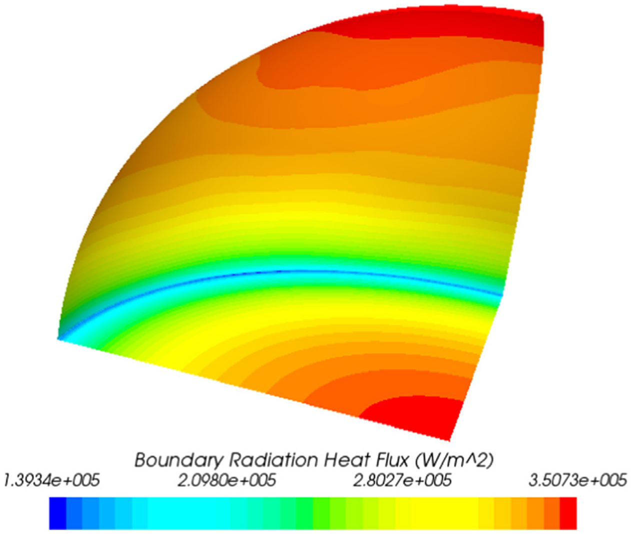

Fig. 6. The radiation heat transfer flux on the wall of the CFD simulation result with the SNB model for case 2.

The CFD simulation with the gray gas model predicts the net heat transfer rate 7.72% higher than that of the manual calculation because the CFD simulation under predicts the gas absorption of the radiation from the wall. In CFD simulation, Eq. (11) is solved once for the whole spectrum, the average absorption coefficient k is used for both the absorption term (left side of the equation) and the emission term (right side of the equation). The real spectral absorption coefficient of course is equal to the spectral emission coefficient, however, the spectrally averaged absorption coefficient is normally not equal to the spectrally averaged emission coefficient since the spectral distribution of the gas emission (spectrally discrete distribution) is not equivalent or proportional to the incident radiation from the wall (spectrally continuous distribution). A better treatment would be using different average coefficients for the left term and right term of Eq. (11) in a CFD simulation, however, this kind of treatment is not implemented in the commercial software currently. Since $\varepsilon_g = 0.4323 < \alpha_g = 0.5658$, it is natural that the CFD simulation under predicts the gas absorption of the incident radiation from the wall.

The CFD simulation with the gray gas model predicts the similar wall radiation heat transfer flux distribution to that of case 1 but with lower value because the wall irradiates now. The CFD simulation with the SNB model gives the same net heat transfer rate as that of the manual calculation showing its superiority over the CFD simulation with the gray gas model. Considering the heat flux result of the SNB simulation to be accurate, then the CFD simulation with the gray gas model over predicts the heat flux by 5–12% for this case.

Case 3. The condition is the same as in case 2 except that the wall is now gray surface with 0.5 emissivity. The manual calculation with the gray gas model is only applicable for the heat transfer between gas and blackbody surface and it cannot be used for this case.

CFD simulation with the gray gas model: $k = 0.2831\ \text{m}^{-1}$, net heat transfer rate to the wall = 13.538 MW, maximum heat flux = 0.2534 MW/m^2, minimum heat flux = 0.1535 MW/m^2, heat flux at the base center = 0.2513 MW/m^2 (Fig. 7).

CFD simulation with the SNB model: net heat transfer rate to the wall = 11.21 MW, maximum heat flux = 0.20524 MW/m^2, minimum heat flux = 0.12823 MW/m^2, heat flux at the base center = 0.20314 MW/m^2 (Fig. 8).

The CFD simulation with the gray gas model over predicts both the heat transfer rate and heat flux by 21% compared to the simulation with the SNB model. With the gray wall, part of the incident gas radiation will be reflected and pass through the gas again. The reflected radiation will be absorbed partially when it goes through the gas, this absorption will be strong since the reflected radiation intensity has the same spectral distribution as the gas irradiation. The gray gas model under predicts this radiation reabsorption causing the over prediction of heat transfer flux and net heat transfer rate.

Case 4. The geometry and pressure are the same as the cases above. The gas is the combustion product of CH_4 burning with 25% excess air now: 2400 K, 7.7% CO_2, 15.4% H_2O, 3.86% O_2, and 73% N_2. The wall is gray surface with temperature 1273 K and emissivity 0.65.

CFD simulation with the gray gas model: net heat transfer rate to the wall = 15.5 MW, maximum heat flux = 0.2988 MW/m^2, minimum heat flux = 0.1599 MW/m^2, heat flux at the base center = 0.292 MW/m^2 (Fig. 9).

CFD simulation with the SNB model: net heat transfer rate to the wall = 12.62 MW, maximum heat flux = 0.2378 MW/m^2, minimum heat flux = 0.1314 MW/m^2, heat flux at the base center = 0.235 MW/m^2 (Fig. 10).

The gray gas model over predicts both the heat transfer rate and heat transfer flux by 23% compared to the SNB model because of the same reason as in case 3, i.e., the gray gas model under predicts the radiation reabsorption.

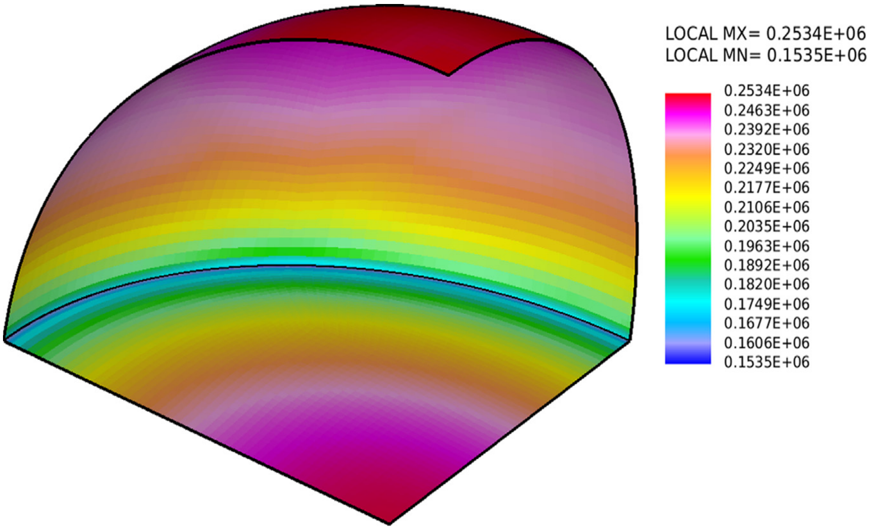

Fig. 7. The radiation heat transfer flux on the wall of the CFD simulation result with the gray gas model for case 3.

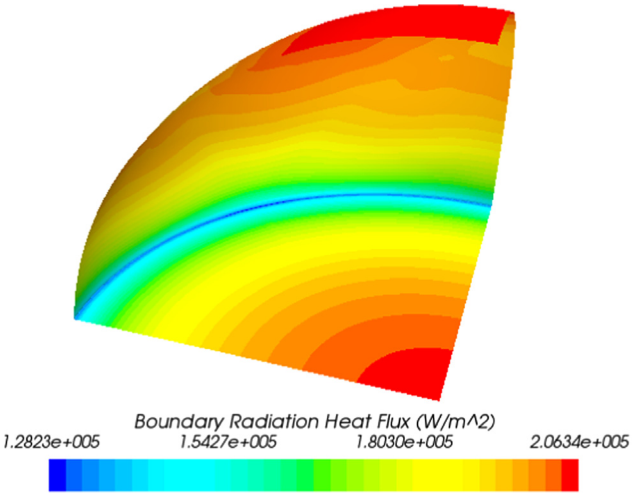

Fig. 8. The radiation heat transfer flux on the wall of the CFD simulation result with the SNB model for case 3.

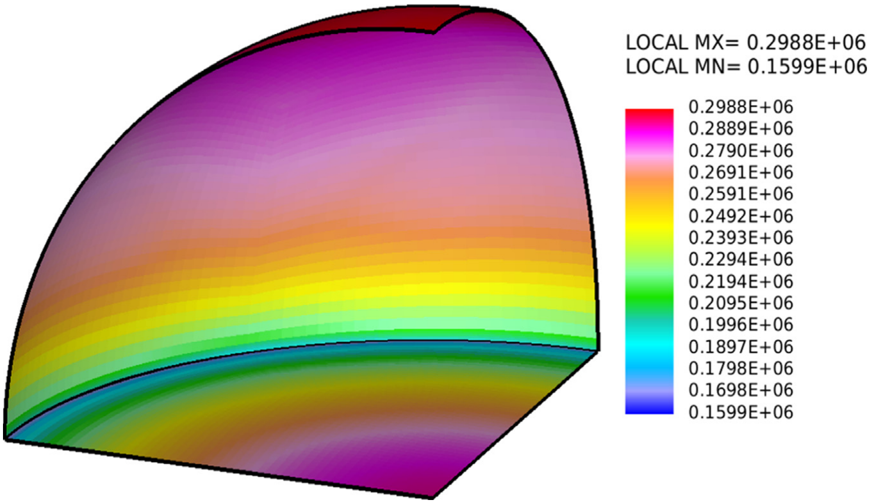

Fig. 9. The radiation heat transfer flux on the wall of the CFD simulation result with the gray gas model for case 4.

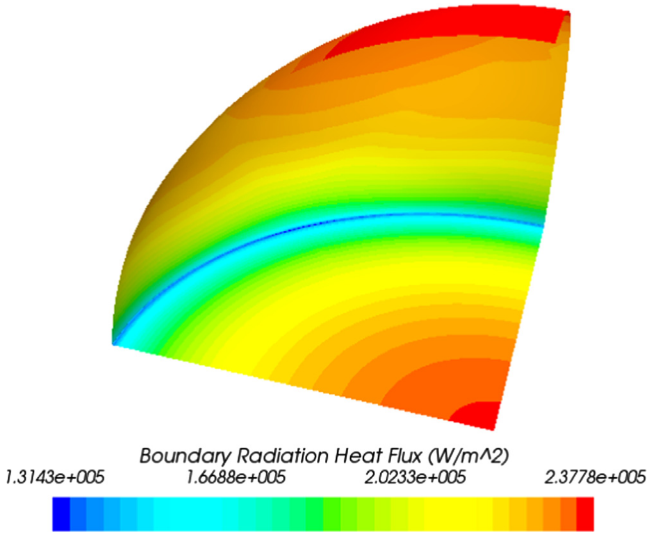

Fig. 10. The radiation heat transfer flux on the wall of the CFD simulation result with the SNB model for case 4.

In summary, for the ideal case 1, the wall is blackbody at 0 K, only the gas radiation exists; the gray gas model predicts the overall gas emission pretty accurate (1.2% relative error). For case 2, the gas radiation is the same as in case 1; but the wall is blackbody surface at 1273 K now, it emits radiation and its emission will be absorbed partially by the gas; the gray gas model under predicts this absorption causing the heat transfer rate over predicted by 7.72%. On the other hand, compared to the accurate SNB model, the gray gas model predicts the relative heat transfer flux distribution correctly: the maximum heat transfer flux locates at the top center of the spherical surface, it gradually diminishes to the minimum value at the edge of the spherical surface and the base plane, then it gradually increases while approaching the center in the base plane (this relative distribution holds for cases 3 and 4, and the gray gas model predicts correct trend for these cases too). However, the gray gas model over predicts the value of the heat transfer flux quantitatively. Cases 3 and 4 are more realistic since the wall is gray surface which will emit radiation and reflect gas radiation; the gray gas model under predicts the gas absorption of both wall emission and reflected gas radiation causing the over prediction of heat transfer rate and flux by 21% in case 3 and 23% in case 4 respectively. However, ~20% prediction error is generally considered good in industry simulations. Artificial increase of the mean radiation beam length could reduce this systematic simulation error.

6. Conclusions

CFD simulation with the gray gas model is frequently used in industrial furnace application because of its efficiency. The accuracy of this method for combustion product radiation calculation has been evaluated by the simulations with the SNB model. It is shown that the gray gas CFD method can predict the relative radiation heat transfer flux distribution correctly. However, it over predicts the radiation heat transfer flux and total heat transfer rate quantitatively because it predicts the gas emission well but under predicts the absorption of wall radiation and the reabsorption of reflected gas radiation. For the tested cases, the error is within 23% and this error should be considered as systematic error of this method.

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