

Study on the radiative transfer through non-gray gas mixtures within an irregular 3-D enclosure by using the modified weighted sum of gray gas method[†]

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Abstract

In this study the modified weighted sum of gray gases model (WSGGM) using the gray gas regrouping technique and the discrete ordinates interpolation method (DOIM) are applied to analyze the radiative transfer within an irregular 3-D enclosure filled with non-gray gas mixture of CO₂, H₂O and N₂. The computer code developed in this study is successfully applied for solving the non-gray gas radiation within a 3-D rectangular enclosure and the gray gas radiation within an irregular 3-D enclosure by showing fairly good agreements with the existing results. In this paper the radiative transfer within an irregular 3-D enclosure filled with non-isothermal non-gray gases with uniform mixtures of CO₂, H₂O and N₂ is studied to demonstrate the applicability of the modified sum of gray gases model for irregular systems and to examine the effect of the concentrations of CO₂ and H₂O on the radiative transfer within modern combustors. Results show that the wall heat fluxes and the radiative heat source terms are increased as the concentrations of CO₂ and H₂O are increased. Results also show that the radiative fluxes caused by the mixture gases with high concentrations CO₂ and H₂O which can be observed in oxy-fuel combustion systems can reach up to nearly twice of those found in ordinary air-fuel combustion systems.

Keywords: Radiative transfer; Non-gray gases; Modified WSGGM; DOIM; Irregular enclosure

1. Introduction

Various industrial thermal applications such as furnaces, boilers, gas turbines and engines utilize the energy from fuel burning by which the heat of combustion and burned gases are generated. Among the burned gases produced from most of the fossil fuels, gaseous CO₂ and H₂O are the major components participating in the radiative heat transfer. Because most of the heat of combustion is transferred radiatively through the processes of absorption, emission and scattering by such high temperature gaseous media, the radiative transfer needs to be analyzed by using more accurate tools while the heat transfer by conduction and convection can be neglected or analyzed by using simplified models. Although the radiative transfer process depends on the various parameters such as wavelength, temperature, pressure and path length etc. the wavelength dependency of the radiative transfer through non-gray gas media is one of the most important phenomena among others.

Since the gaseous CO₂ and H₂O are the typical non-gray gases appearing in the fossil-fuel fired combustors which have

strongly wavelength dependent properties in absorption and emission of the radiation energy, development of proper modeling tools for the radiative properties of non-gray gases is very important. Radiative property models for non-gray gases explained in many text books are the line-by-line models, the band models and the global models, where the line-by-line models result in accurate spectral properties with large computational load but the global models show less accurate results with minor computational load. Among the global models, the weighted sum of gray gases model (WSGGM) introduced by Hottel and Sarofim [1] is fairly well developed to have merits in accuracy and computational load. Modest [2] showed that the WSGGM was applicable with any desired solution methods and generally model constants provided by Smith et al. [3] are used. Kim and Song [4, 5] developed a narrow band based WSGGM to solve radiative transfer through nongray gas media with uniform gas concentrations. Park and Kim [6, 7] modified the narrow band based WSGGM for arbitrary mixtures of CO₂ and H₂O gases and improved the computational efficiency of the WSGGM for gas mixtures by using the gray gas regrouping process which was performed by comparing the magnitudes of the gray gas absorption coefficients.

In the radiative transfer analysis using non-orthogonal grids Chui and Raithby [8] were successful analyzing the radiative

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transfer within two-dimensional trapezoidal, annular and J-shaped regions by using the finite volume method (FVM). Also Kim and Baek [9] were successful analyzing the radiative transfer within a three-dimensional gas turbine shaped furnace by using the FVM. The discrete ordinate interpolation method (DOIM) proposed by Cheong and Song [10] for two-dimensional system doesn't use the control volume concept instead they considered the radiative transfer along lines of sight starting from the system walls. Seo and Kim [11] extended the DOIM to 3-D systems by using triangular interpolation planes. Recent studies on radiative transfer using 3-D non-orthogonal grids are focused on various interpolation methods [12, 13].

The purpose of this study is to analyze the radiative transfer in a non-orthogonal 3-D enclosure filled with non-gray gas mixtures of CO₂ and H₂O. The non-gray gas property is modeled by using the modified WSGGM proposed by Park and Kim [7] and the radiative transfer analysis by using the non-orthogonal grids is performed by using the 3-Dimensional DOIM [11]. A 3-D hexahedral system surrounded by flat quadrangles which is the same one as used by Cha [12] is considered in this study. Non-gray gas media considered in this study are mixtures of CO₂, H₂O and N₂ and presume uniform concentrations and non-isothermal distribution [7, 14] within the system. Especially the range of CO₂ and H₂O concentrations is covered up to those encountered by the oxy-fuel combustion systems.

2. Radiative transfer equation

For an absorbing, emitting, and scattering medium, the radiative transfer equation can be expressed as follows for an infinitesimal path length Δs shown in Fig. 1. Assuming the extinction coefficient is constant over the path length (Δs) as β(s) ≈ β_p, the radiative transfer equation can be expressed in the following approximate form [8].

$$I_p(\Omega) \approx I_u(\Omega)e^{-\beta_p \Delta s} + \frac{S_p(\Omega)}{\beta_p}(1 - e^{-\beta_p \Delta s}) - \frac{1}{\beta_p^2} \left(\frac{\partial S(s, \Omega)}{\partial s} \right)_p \{1 - e^{-\beta_p \Delta s} (1 + \beta_p \Delta s)\} \tag{1}$$

Where I_u is the radiative intensity at the upstream node (u) along the Ω direction. The source function S_p(Ω) is expressed as following.

$$S_p(\Omega) = aI_{pb} + \frac{\sigma_s}{4\pi} \int_{4\pi} I(\Omega') \Phi(\Omega'; \Omega) d\Omega' \tag{2}$$

Where β_p in Eq. (1) is the extinction coefficient the medium which is the sum of the absorption coefficient (a) and the scattering coefficient (σ_s). I_{pb} is the black body intensity at point P and Φ(Ω'; Ω) is the medium scattering phase function.

The DOIM [11] is a method that computes the radiative in-

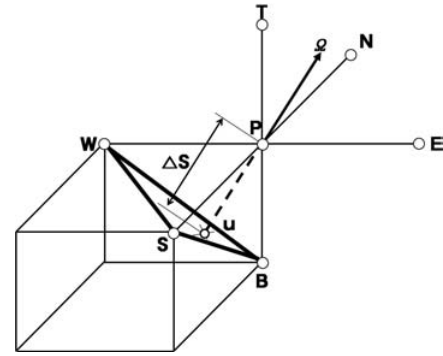


Fig. 1. Triangular interpolation plane and change of the radiative intensity along a path.

tensity at point P by using Eq. (1) with the upstream radiative intensity at point u which is linearly interpolated by using the intensity values at W, S and B as shown in Fig. 1. In this method, the angular distribution of the radiative intensity at point P is determined at the designated discrete angular ordinates [11].

3. Modified weighted sum of gray gases model (WSGGM)

The hypothesis that the spectra of two absorbing gases in a narrow band are uncorrelated is generally accepted and holds for CO₂-H₂O mixtures with fairly good accuracy [15, 16]. Then the transmittance of the gas mixture of CO₂ and H₂O (τ_{mix}) over a narrow band along the wave length (η) can be expressed as a multiplied sum of the individual transmittance of each gray gas [4, 5].

$$\overline{\tau}_{mix}(\eta) = \sum_{ic=1}^{M_{CO_2}} \sum_{ih=1}^{M_{H_2O}} W_{ic,CO_2}(\eta) \times W_{ih,H_2O}(\eta) e^{-(\kappa_{ic,CO_2} + \kappa_{ih,H_2O})} \tag{3}$$

Where W_i(η) is the spectral weighting factor for the ith gray gas (CO₂ and H₂O), M is the number of gray gases to represent each of the non-gray gas (CO₂ and H₂O) and κ_i is the ith gray gas absorption coefficient.

The narrow band transmittance of the mixture gas with path length L can also be expressed as following

$$\overline{\tau}_{mix}(\eta) = \sum_{i=1}^{M_{mix}} W_{i,mix}(\eta) e^{-\kappa_{i,mix} L} \tag{4}$$

Where the number of gray gases required for the mixture gas (M_{mix}) is equal to the multiplication of M_{CO₂} and M_{H₂O}. The spectral weighting factor (W_{mix}) and the absorption coefficient (κ_{mix}) for the mixture gas can also be determined as following [5].

$$W_{mix}(\eta) = W_{CO_2}(\eta) \times W_{H_2O}(\eta) \tag{5}$$

$$\kappa_{mix} = \kappa_{i0,CO_2} \frac{e^{-\alpha_{i,CO_2}/T}}{T^2} PX_{CO_2} + \kappa_{i0,H_2O} \frac{e^{-\alpha_{i,H_2O}/T}}{T^2} PX_{H_2O} \tag{6}$$

Where κ_{i0} and α_i are modeling constants for the ith gray

gas and P , T , X are pressure, temperature and molecular weight.

The required number of gray gases for the narrow band based WSGGM becomes very large to represent the radiative characteristics of non-gray mixture gases. In order to improve the computational efficiency of the WSGGM applied for gas mixtures, Park and Kim [7] proposed a gray gas regrouping process. The gray gas regrouping process is performed by comparing the magnitude of the gray gas absorption coefficients where it is subdivided into a pre-specified number of M_{new} groups [7]. In this model M_{new} becomes the new number of gray gases and the corresponding model is named as $RG - M_{new}$. The new weighting factor for the i^{th} gray gas group is obtained by simply summing up the original weighting factors of the gray gases [7].

$$W_{i,new}(\eta) = \sum_{j=1}^{N_i} W_{j,mix}(\eta) \quad (7)$$

Where N_i is the number of gray gases in the i^{th} group and the parameters with the subscript new indicate that they are regrouped parameters. The new absorption coefficient for the i^{th} gray gas group, $\kappa_{i,new}$ can be expressed in the form of Planck mean type as following [7].

$$\kappa_{i,new} = \frac{\sum_{j=1}^{N_i} \kappa_{j,mix} W_{j,mix}}{W_{i,new}} \quad (8)$$

In absorbing, emitting and non-scattering media the radiative transfer equation of the i^{th} gray gas is expressed by using Eq. (1) as following.

$$\begin{aligned} I_{pi}(\Omega) \approx & I_{ui}(\Omega) e^{-\kappa_{pi,new} \Delta s} \\ & + \frac{\kappa_{pi,new} W_{pi,new} I_{pb}(\Omega)}{\kappa_{pi,new}} (1 - e^{-\kappa_{pi,new} \Delta s}) \\ & - \frac{1}{\kappa_{pi,new}^2} \left\{ 1 - e^{-\kappa_{pi,new} \Delta s} (1 + \kappa_{pi,new} \Delta s) \right\} \times \\ & \frac{\kappa_{pi,new} W_{pi,new} I_{pb}(\Omega) - \kappa_{ui,new} W_{ui,new} I_{ub}(\Omega)}{\Delta s} \end{aligned} \quad (9)$$

Then the total intensity $I_p(\Omega)$ is then obtained by simply summing up each of the gray gas intensity over the new regrouped number of gray gases (M_{new}) as

$$I_p(\Omega) \approx \sum_{i=1}^{M_{new}} I_{pi}(\Omega) \quad (10)$$

4. Validation of the method proposed; non-gray gas radiation within a rectangular parallelepiped

To validate the method proposed in this paper, the computer code developed to ingrate the modified WSGGM [6, 7] and the DOIM [11] is applied to some previous problems reported

Table 1. Conditions applied for non-gray gases in the rectangular parallelepiped [14].

| Temperature distribution | Gas mixture compositions |
|--|---|
| Non-uniform $\frac{(x-x_{cen})^2}{a^2} + \frac{(y-y_{cen})^2}{b^2} < 1 :$ $T(x,y,z) = [T_{cen}(z) - 800] f(x,y) + 800$ $\frac{(x-x_{cen})^2}{a^2} + \frac{(y-y_{cen})^2}{b^2} > 1 :$ $T = 800$ | uniform, $CO_2/H_2O/N_2$ mixture $0.2H_2O + 0.1CO_2 + 0.7N_2$ |

Walls are black and cold at 300 [K]
 The pressure of the gas mixture in the enclosure is kept at 1 [atm]

x_{cen} = center of x axis, y_{cen} = center of y axis
 $a = L_x/2$, $b = L_y/2$
 $L_x = 2$ [m], $L_y = 2$ [m], $L_z = 4$ [m], $z_k = 0.375$
 $z < z_k$: $T_{cen}(z) = 1400z/z_k + 400$
 $z \geq z_k$: $T_{cen}(z) = 1000(L_z - z)/(L_z - z_k) + 800$

$$f(x,y) = 1 - 3 \left(\sqrt{(x-1)^2 + (y-1)^2} \right)^2 + 2 \left(\sqrt{(x-1)^2 + (y-1)^2} \right)^3$$

in the literature. A 3-D rectangular system of 2 [m] × 2 [m] × 4 [m] surrounded by cold black walls which is filled with non-gray gas mixture of CO_2 and H_2O is considered for this purpose and the results are compared with preliminary study [14]. The non-gray gas medium considered is assumed to have a uniform concentration and non-isothermal temperature distributions as explained in Table 1. The computational grids of $17 \times 17 \times 24$ are used to solve the problem with uniform grids in the x and y directions and with non-uniform grids in the z direction where finer grids are placed around the location of the peak gas temperature near $z=0.375$ [m] [14].

Results shown in Fig. 2 and 3 are the S8 solutions obtained by using the discrete ordinate method (DOM) [7, 14] and the current DOIM applied with the modified WSGGM. Fig. 2 shows the wall heat flux [kW/m²] along the z axis at $x=1$ [m] and $y=2$ [m], and the wall heat fluxes obtained by using the current method with $M_{new} = 8$ ($RG - 8$) agree fairly well with the results presented by Liu [14] within 3.4% difference. Fig. 3 shows the radiative heat source term [$-\nabla \cdot \vec{q}_r$, kW/m³] along the z axis at $x=1$ [m] and $y=1$ [m], the radiative heat source term results obtained by using the current method with $M_{new} = 8$ ($RG - 8$) agree fairly well with the results presented by Liu [14] within 13% difference. The differences appeared in the wall heat fluxes and the radiative heat source terms between the results of Liu and those of the current method with $M_{new} = 12$ ($RG - 12$) are reduced to within 3.0% and 5.7% differences.

5. Validation of the method proposed; gray gas radiation within a non-orthogonal hexahedron

The results obtained by using the current method are also compared with the solutions obtained from non-orthogonal systems filled with a gray gas appearing in the literature. In

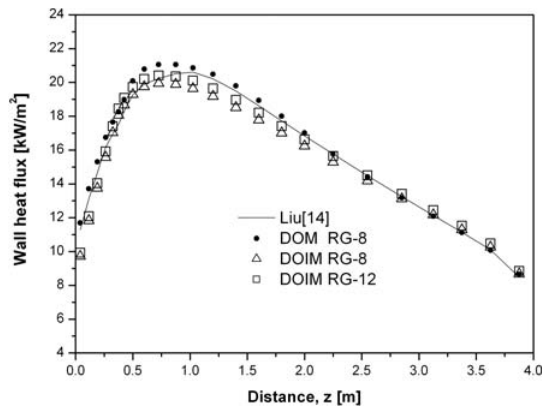


Fig. 2. Comparison of the wall heat fluxes along the z-axis at $x=1$ [m], $y=2$ [m] for different solution methods.

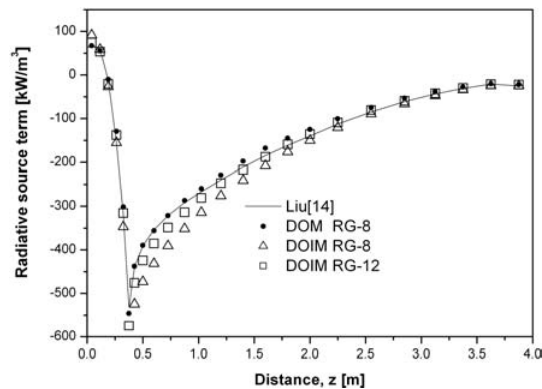


Fig. 3. Comparison of the radiative heat source terms along the z-axis at the centerline for different solution.

this study, the non-orthogonal hexahedral enclosure considered by Cha and Song [12] is utilized to demonstrate the applicability of the computer code developed in this study. Fig. 4 shows the outline of the hexahedral enclosure where all of the system walls are assumed to be cold black, and it is assumed that the hexahedral enclosure is filled with isothermal gray gases at an absolute temperature of T . Although the computational grids of $11 \times 11 \times 11$ are used to obtain the exact solutions in [12], we tested two different grids of $11 \times 11 \times 11$ and $21 \times 11 \times 21$ to examine the grid dependency of the method used in this study.

In Fig. 5, the non-dimensional wall heat fluxes along W-W for different absorption coefficient (κ) of the gray gases obtained from the computer code developed in this study with the DOIM are compare with the exact solutions provided by Cha and Song [12]. The results obtained from our computer code show fairly good agreements with the exact solutions of Cha and Song [12] for both of the grid systems tested; by showing the average errors of 3.23% for $\kappa = 10$ [m^{-1}], 7.37% for $\kappa = 1$ [m^{-1}] and 9.25% for $\kappa = 0.1$ [m^{-1}] for $11 \times 11 \times 11$ grids and by showing the average errors of 1.72% for $\kappa = 10$ [m^{-1}], 6.07% for $\kappa = 1$ [m^{-1}] and 6.28% for $\kappa = 0.1$ [m^{-1}] for $21 \times 11 \times 21$ grids respectively. The results show that the method used in this study may result in

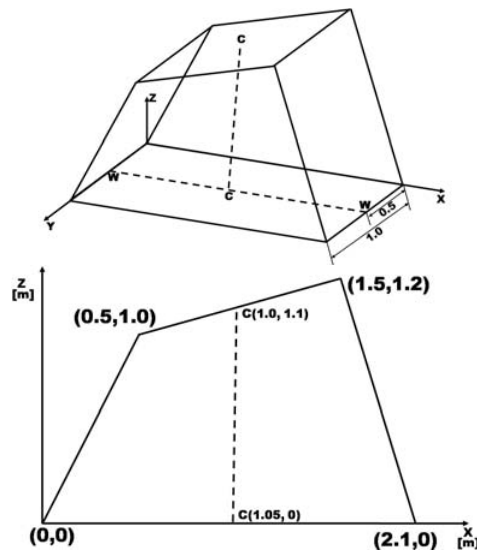


Fig. 4. Hexahedral enclosure considered [12].

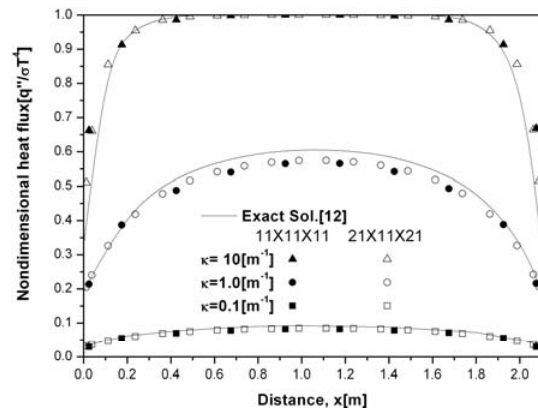


Fig. 5. Non-dimensional wall heat fluxes along the x-axis at W-W for gray gases.

fairly good solutions for the radiative transfer problems in the non-orthogonal hexahedron with the $21 \times 11 \times 21$ grids.

6. Solutions for non-orthogonal hexahedron filled with non-gray gases

The computer code developed for solving the radiative transfer problems within non-orthogonal 3-D enclosures filled with non-gray gases is now applied for a non-orthogonal hexahedron shown in Fig. 4 filled with non-gray gases of arbitrary mixtures of CO_2 , H_2O and N_2 . The computational grids of $21 \times 11 \times 21$ are considered to obtain accurate solutions. The temperature distribution within the system is assumed to be expressed as the same numerical expression as shown in Table 1 and the geometric data used for the numerical expression applied for the non-orthogonal hexahedron considered here are summarized in Table 2. As shown in Table 2, four different mixture gases with different ratios of CO_2 , H_2O and N_2 are considered to obtain the radiative transfer solutions. Especially mixture gases with high CO_2 and H_2O concentrations are also

Table 2. Conditions applied for non-gray gases in the non-orthogonal hexahedron.

| Temperature distribution | Gas mixture compositions |
|--|---|
| Walls are black and cold at 300 [K] Equations in Table 1 are applied. $L_x = 2.1$ [m], $L_y = 1$ [m], $L_z = 1.2$ [m], $z_k = 0.1125$ | 4 different mixture gases with uniform spatial distribution $0.1H_2O + 0.1CO_2 + 0.8N_2$ $0.1H_2O + 0.2CO_2 + 0.7N_2$ $0.2H_2O + 0.1CO_2 + 0.7N_2$ $0.6H_2O + 0.3CO_2 + 0.7N_2$ |

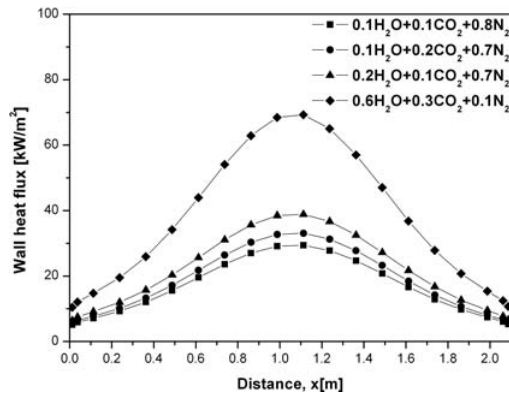


Fig. 6. Comparison of the wall heat fluxes along the x-axis at W-W for non-gray gas mixtures.

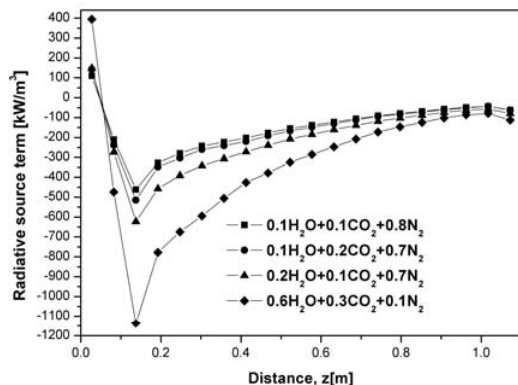


Fig. 7. Comparison of the radiative heat source terms along the z-axis at C-C for non-gray gas mixtures.

considered to simulate the situations appeared in many recent oxy-fuel combustion systems of growing concern.

Fig. 6 shows the wall heat flux distribution along the x-axis at W-W as shown in Fig. 4 for four different mixture gases with different concentrations of H_2O , CO_2 and N_2 . Results show that the wall heat fluxes are increased as the concentrations of CO_2 and H_2O are increased. At $x=1.05$ [m], the gas temperature has a peak value and the wall heat flux distributions show peak distributions near this location. The peak wall heat fluxes obtained from the mixture gases of $0.1H_2O+0.2CO_2$ and $0.2H_2O+0.1CO_2$ are 12.5% and 32.2% higher than that of $0.1H_2O+0.1CO_2$ showing that the H_2O is the more important absorbing medium as compared to the CO_2 . The mixture gas of $0.3CO_2+0.6H_2O$ shows the peak wall heat flux up to 78.4% higher than that of $0.2H_2O+0.1CO_2$

which is usually appeared in the air-fuel combustion systems.

Fig. 7 shows the radiative heat source term ($-\nabla \cdot \vec{q}_r$) along the z-axis at C-C as shown in Fig. 4 for four different mixture gases with different concentrations of H_2O , CO_2 and N_2 . Results show that the radiative heat source terms are increased as the concentrations of CO_2 and H_2O are increased as observed for the wall heat flux distributions. The peak radiative heat source terms obtained from the mixture gases of $0.1H_2O+0.2CO_2$ and $0.2H_2O+0.1CO_2$ are 11.6% and 34.9% higher than that of $0.1H_2O+0.1CO_2$. The mixture gas of $0.3CO_2+0.6H_2O$ shows the peak radiative heat source term up to 82.6% higher than that of $0.2H_2O+0.1CO_2$ representing air-fuel combustion systems.

7. Conclusions

In this study the modified weighted sum of gray gases model (WSGGM) and the discrete ordinates interpolation method (DOIM) are applied to analyze the radiative transfer within an irregular 3-D enclosure filled with non-gray gas mixtures of CO_2 , H_2O and N_2 . The modified weighted sum of gray gases model (WSGGM) is used together with the gray gas regrouping technique. The computer code developed in this study is successfully applied for solving the non-gray gas radiation within rectangular and irregular 3-D enclosures. In the rectangular enclosure results have an acceptable maximum difference of 3.5% in wall heat fluxes as compared to the previous solutions reported in the literature. And in the irregular 3-D enclosure filled with gray gas results show fairly good agreements with the exact solutions reported in the literature by showing about 6% maximum error in wall heat fluxes. In order to demonstrate the applicability of the modified weighted sum of gray gases model (WSGGM) for irregular system, we consider an irregular 3-D enclosure to examine the effect of the concentrations of CO_2 and H_2O . Results show that the wall heat fluxes and the radiative heat source terms are increased as the concentrations of CO_2 and H_2O are increased. Especially the radiative fluxes caused by the combustion mixture gases with very high concentrations of CO_2 and H_2O which can be observed in many oxy-fuel combustion systems can reach up to nearly twice of those found in ordinary air-fuel combustion systems. The weighted sum of gray gases model (WSGGM) with gray gas regrouping technique introduced in this study can be a useful engineering tool in modeling the radiative transfer problems within irregular enclosures filled with non-gray gas mixtures while the more accurate narrow band model is limited due to the large computing load.

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