Numerical Simulation of Combustion and Nongray Radiative Heat Transfer in a Furnace and Its Comparison with Experiments*

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Numerical simulations of heat transfer in a furnace of practical scale were carried out, coupled with a prediction of the flame. Radiative heat transfer was computed taking its nongray characteristic into account. Convective heat transfer to the furnace wall was incorporated as well. The numerical computations were conducted based upon the conservation equations of mass, momentum, energy and species together with the k - ϵ turbulence model and the eddy dissipation model for estimating the combustion rate and the effective viscosity. Radiative heat transfer was computed using the radiant heat ray method in combination with a weighted-sum-of-gray-gas model or a wide-band model. Predicted results were compared with experimental data. Comparisons showed that the profiles of temperature and species concentration can be predicted fairly well and that the weighted-sum-of-gray-gas model as well as the wide-band model gives a good prediction of heat flux to the furnace wall. The influence of soot on furnace heat transfer was also estimated.

Key Words: Radiative Heat Transfer, Nongray Analysis, Combustion, Furnace, Numerical Simulation

1. Introduction

Heat transfer to the furnace wall is one of the important features in estimating furnace performance. Heat transfer includes radiative and convective heat transfer. Both of which are crucially influenced by the profiles of gas temperature and species concentration in the furnace. Such profiles are dominated by flow pattern and flame configuration. So, in order to obtain a well-grounded prediction of furnace heat transfer, radiative and convective heat transfer should be estimated in combination with proper predictions of flow and combustion in the

furnace.

Radiative heat transfer from the flame has been extensively studied. Pioneering studies are summarized in Refs.(1) and (2). However, it is difficult to clarify the relationship between emissivity and thickness of the gas layer. Relatively recent studies are described in Refs.(3) to (5), which stress the nongray radiative properties of gaseous molecules and their physical models.

The peculiar feature of radiative heat transfer, which requires the treatment of three-dimensional far-field exchange of energy, makes its quantitative estimation complex. Moreover, the nongray characteristic of gaseous radiation increases the computational load. Recent developments in computer and computation algorithms, however, have made the problem tractable. Numerical computations of radiative heat transfer together with flow and combustion have been made in turbulent axisymmetric boundary-layer-type diffusion flames, using the radiant heat ray method. Radiative heat transfer was computed in a three-dimensional large-scale pulverized coal boiler⁽⁶⁾ using the discrete ordinate method. There are, however,

* Received 7th April 1999, Japanese original: Trans. Jpn. Soc. Mech. Eng., Vol. 64, No. 626, B (1998), p. 3391-3397 (Received 7th June, 1996)

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few quantitative comparisons between predictions and experimental data⁽⁶⁾⁻⁽⁹⁾. Moreover, there are even less precedents taking the nongray feature of gaseous radiation into account.

In the present study, the numerical computations of radiative and convective heat transfer to the furnace wall are carried out considering the nongray feature of gaseous radiation, together with the prediction of flow and combustion in a furnace based on fundamental conservation equations. The radiant heat ray method was used to evaluate radiative heat transfer in combination with a weighted-sum-of-gray-gas model⁽²⁾ or a wide-band model⁽¹⁰⁾. Gas temperature, species concentration and heat transfer to the furnace wall are compared with experiments. Also, the influence of soot on the furnace heat transfer is briefly estimated.

2. Configuration of the Flame in a Furnace

The furnace has a water-cooled cylindrical wall, 1 m in inner diameter and 4.8 m in height, and is vertically settled to secure the axial symmetry of the flame. The furnace wall is composed of nine cylindrical segments, each of which is separately cooled with water to obtain an axial profile of heat flux at the wall. The fuel used in this furnace is propane whose purity is above 98 percent. The fuel nozzle is set up coaxially together with the air register at the bottom center of the furnace. Fuel is injected vertically upward along the central axis through the single-hole type of fuel nozzle whose inner diameter is 10 mm. Combustion air is supplied upward coaxially with the fuel through the air register of 260 mm inner diameter. The fuel flow rate is 30 kg/h, and the total air ratio is 2.0. The air temperature at the furnace inlet is 20°C.

The flame formed in this furnace is an axisymmetric turbulent diffusion flame. The flame length is nearly 250 cm, which is of relatively large scale as compared with that of usual laboratory-scale flame.

3. Formulation and Models

3.1 Fundamental equations

An axisymmetric turbulent diffusion flame is formed in a cylindrical furnace. Cylindrical coordinates are used. The fundamental equations formulated here are of the elliptic type to allow for reverse flow regions. The conservation equations for mass, momentum, species, energy, kinetic energy of turbulence and its dissipation rate are expressed in the following unified form.

$$\begin{aligned} & \frac{\partial}{\partial t}(\rho\phi) + \frac{\partial}{\partial x}(\rho U\phi) + \frac{1}{r} \frac{\partial}{\partial r}(r\rho V\phi) \\ & = -\frac{\partial}{\partial x}\left(b\frac{\partial\phi}{\partial x}\right) + \frac{1}{r} \frac{\partial}{\partial r}\left(r b \frac{\partial\phi}{\partial r}\right) + S_\phi \end{aligned} \quad (1)$$

ϕ represents various dependent variables such as the axial velocity component, U ; radial velocity component, V ; kinetic energy of turbulence, k ; its dissipation rate, ε ; enthalpy, h ; mass fraction of species i , m_i ; and mixture fraction, f , as shown in Table 1. The effective viscosity is calculated using elsewhere the k - ε 2 equation model⁽¹¹⁾. The exchange coefficients b and the source terms S_ϕ interrelated to each dependent variable in Eq. (1) are also shown in Table 1. In the above equation and Table 1, x and r represent the axial and radial coordinates, respectively; P , pressure; T , temperature; ρ , density; ρ_0 , reference density; μ_e , the effective viscosity; R_i , production rate of i -species by chemical reaction; and Q_r , net heat absorption rate per unit volume through radiative heat transfer. σ_k , σ_ε , σ_h and σ_f are effective Prandtl or Schmidt numbers which are empirical constants to be selected as 1.0, 1.3, 0.7 and 0.7, respectively.

3.2 Models for combustion reaction

As regards the combustion reaction, we take into consideration the following seven species: C_3H_8 , N_2 , O_2 , CO_2 , CO , H_2O and H_2 . According to the concept of the eddy breakup model proposed by Magnussen and Hjertager⁽¹²⁾, the volume of gas in which eddy breakup takes place is proportional to (ε/k) . Assuming that the gas brought into the eddy breakup changes into the reaction product of adiabatic equilibrium composition corresponding to the equivalence ratio of the calculation cell under consideration, the production rate of the i -species R_i is expressed in the following unified form.

$$R_i = A\rho(\varepsilon/k)(m_i^* - m_i) \quad (2)$$

m_i is mass fraction of species i and m_i^* is adiabatic equilibrium mass fraction. The empirical constant A is 4.0⁽¹²⁾.

Table 1 Dependent variables, exchange coefficient and source terms in Eq. (1)

ϕ	b	S_ϕ
1	0	0
U	μ_e	$\frac{\partial}{\partial x}\left(\mu_e \frac{\partial U}{\partial x}\right) + \frac{1}{r} \frac{\partial}{\partial r}\left(\mu_e r \frac{\partial U}{\partial r}\right) - \frac{\partial P}{\partial x} - (\rho - \rho_0)g$
V	μ_e	$\frac{\partial}{\partial x}\left(\mu_e \frac{\partial V}{\partial x}\right) + \frac{1}{r} \frac{\partial}{\partial r}\left(\mu_e r \frac{\partial V}{\partial r}\right) - 2\mu_e \frac{V}{r^2} - \frac{\partial P}{\partial r}$
k	μ_e/σ_k	$G_k - \rho\varepsilon$
ε	μ_e/σ_ε	$\varepsilon(C_1 G_k - C_2 \rho\varepsilon)/k$
h	μ_e/σ_h	R_i
f	σ_e/σ_f	0

3.3 Models for gaseous radiation and absorption

Infrared-active species, such as water vapor and carbon dioxide, have several absorption bands composed of many very closely spaced absorption lines. They absorb radiation energy in such absorption bands and do not absorb it outside such absorption bands. It is unreasonable to treat infrared-active gases as gray ones.

One of the methods for treating the nongray feature is the use of the weighted-sum-of-gray-gas model⁽¹⁾. In this model, a mixture of real gas is represented by the sum of several kinds of gray gas. In each gray band, the relationship between the total emissivity of such a mixture versus the path length L is expressed by Lambert-Beer formula. For the combustion gas containing soot, one approach⁽²⁾ to obtain the total emissivity ϵ_{gs} is proposed as follows.

$$\epsilon_{gs} = \sum_n a_n [1 - \exp(-K_n L)] \quad (3)$$

Here, K_n and the weighting factor a_n of n -th gray gas are expressed as follows.

$$K_n = k_{g,n}(P_{CO_2} + P_{H_2O}) + k_{s,n}\rho m_s \quad (4)$$

$$a_n = a_n + \beta_n T \quad (5)$$

P_{CO_2} and P_{H_2O} are partial pressures of carbon dioxide and water vapor respectively. ρ is density of combustion gas and m_s is mass fraction of soot. The values of a_n , β_n , $k_{g,n}$ and $k_{s,n}$ ⁽²⁾ have been given for the combustion gas containing CO_2 and H_2O at the same partial pressure and soot according to the assumption $n=3$ (This is called the three-gray-gas model). Here, $k_{g,n}$ and $k_{s,n}$ are assumed to be independent of temperature. Absorption coefficients are constant and the temperature dependence is fully accounted for by the weighting factor a_n . T is temperature.

Equation (3) can be interpreted as follows. $1 - \exp(-K_n L)$ is the emissivity of the n -th gray gas. a_n may be interpreted as the fraction of blackbody radiation energy in a spectral region in which the absorption coefficient is K_n . The radiation energy per unit time and the unit volume of the n -th gray gas is expressed as $4\sigma T^4 K_n$. σ is the Stefan-Boltzmann radiation constant. The combustion gas contained in a calculation cell having a volumetric capacity of $V_{i,j}$ emits radiation energy and can be expressed as

$$E_n(i, j) = 4\sigma T^4 V_{i,j} a_n K_n \quad (6)$$

When this radiation energy is absorbed by the same gas, K_n is applied as the absorption coefficient. This interpretation is convenient for computation of the radiative heat transfer using the radiant heat ray method. In this study, the above-mentioned interpretation is extended to nonisothermal and non-homogeneous mixture fields by estimating K_n of the combustion gas based on its temperature and concentration. The absorptivity of the furnace wall is

assumed to be 1.0. The radiation from the furnace wall is neglected because the temperature of the wall is nearly 50°C or lower.

4. Numerical Procedure

The differential equations represented by Eq. (1) together with Table 1 are discretized through a finite difference method. The computational domain is divided into a number of cells. A calculation mesh including 32×39 cells in both radial and axial directions is created. The mesh covers half of the vertical symmetry plane of the furnace with nonuniform cell size. The size of the grid cells adjacent to the fuel nozzle is refined. The size of the grid cells downstream is rough. All discretized equations are solved in a fully coupled form. Converged solutions are obtained by iterative computations using the SIMPLER algorithm⁽¹³⁾ in combination with the radiant heat ray method⁽⁸⁾ used for estimating the magnitude of net radiative absorption which appears in the source term of the conservation equation of energy.

Boundary conditions are specified as follows. At the exit of the fuel nozzle, the radial profiles of axial velocity, turbulent kinetic energy and its dissipation rate are determined assuming that the flow in the fuel nozzle is a fully developed turbulent flow. At the exit of the air register, axial velocity and relative turbulence intensity are given flat radial profiles and the dissipation rate, ϵ , is assumed to be in partial equilibrium with the turbulence kinetic energy. The radial component of velocity is assumed to be zero at the exit of the fuel nozzle and the air register. At the boundary on the axis of symmetry, the radial gradient is assumed to be zero in relation to all the dependent variables except for the radial component of velocity. The radial component of velocity is assumed to be zero on the same boundary. At the boundary downstream of the diffusion flame, the radial component of velocity is also assumed to be zero, and the axial gradient is assumed to be zero in relation to all the dependent variables except for the radial component of velocity. On the furnace wall, wall function methods are applied to axial velocity U , turbulence kinetic energy k and its dissipation rate ϵ . The convective heat transfer to the wall is also evaluated using a wall function method⁽¹⁴⁾.

The computational procedures are illustrated in Fig. 1 in the form of a flow diagram. Prior to the start of calculation, the initial conditions, that is, the estimated profiles of all dependent variables, are specified. The fundamental equations are solved through iterations in the first stage to obtain the profiles of velocity, species concentration and temperature in the furnace. Radiative heat transfer is not incorporated in the first

Fig. 1 Computation flow chart

stage.

In the second stage, the computation of radiative heat transfer using the radiant heat ray method⁽⁸⁾ is carried out on an identical calculation mesh that is used in discretizing the fundamental equations. In this stage, the net absorption of radiative energy by each calculation cell is evaluated by using values of temperature and species concentration computed in the first stage. This net absorption of radiative energy leads to the source term Q_r in the conservation equation of energy. Using this renewed source term Q_r , iterations of the combined first and second stage are conducted to obtain the totally converged solution incorporating radiative heat transfer. The nongray gas is replaced by three gray gases for which the heat transfer rates are calculated independently. The number of beams from each calculation cell is 300.

5. Computed Results and Comparisons with Experiments

5.1 Profiles of species concentration

The computed radial profiles of species concentration in the cross sections at $L=50$ and 250 cm are compared with corresponding experimental data in Figs. 2 and 3. L is the axial distance from the fuel nozzle tip, and R is the radial distance from the

(a) Computation

(b) Experiment

Fig. 2 Radial profiles of species concentration ($L=50$ cm)

central axis of the furnace. Figures 2(a) and 3(a) are the computed results and Figs. 2(b) and 3(b) are the measured ones.

By observing the concentration profiles in the cross section of $L=50$ cm, the predicted results in Fig. 2(a) indicate the following. The concentration of C_3H_8 exhibits a maximum value on the central axis. The concentration of combustion products such as CO_2 and H_2O takes a maximum value at the radial position slightly away from the central axis. According to the experimental results, a luminous flame zone is observed at this radial location. The radial location of the maximum concentration of intermediate species such as CO and H_2 deviates slightly toward the central axis from those of CO_2 and H_2O . The experimental results shown in Fig. 3(b) include also the

(a) Computation

(b) Experiment

Fig. 3 Radial profiles of species concentration ($L=250$ cm)

concentration profiles of hydrocarbon species such as C_2H_4 , C_2H_6 , C_3H_6 , and CH_4 that are cracked from C_3H_8 . Though some of these cracked hydrocarbon species do not exhibit a maximum value on the central axis, the measured profiles of C_3H_8 and the total hydrocarbon exhibit a maximum value on the central axis. The concentration profiles of other species also show a quantitative tendency similar to the predicted results. Moreover, the relationship among the radial locations where the concentration of CO_2 , H_2O , CO and H_2 takes a maximum value observed in the predicted results is similar to that in the experiment.

In the case of the cross section at $L=250$ cm, the concentration profiles are flat and little hydrocarbon species is detected; the residual combustible species

Fig. 4 Radial profiles of temperature. (a) Computation (long and short dashed lines: without radiative contribution, broken lines: with gaseous radiation only, solid lines: with gaseous and soot radiation), (b) Experiment

are CO and H_2 , as shown in Fig. 3. The concentration profiles in this cross section are also predicted quantitatively well.

5.2 Profiles of temperature

Figure 4(a) shows the radial profiles of temperature in the four cross sections, which were computed using the weighted-sum-of-gray gas model. The alternating long and short dashed lines indicate the temperature computed without radiative heat transfer. Temperature computed considering only gaseous radiation is shown by broken lines. Temperatures computed including also the contribution of soot to the radiative heat transfer are shown by solid lines. The predicted profiles of soot concentration are shown in Fig. 5. The rate was determined by intermixing in a molecular scale of fuel and oxygen eddies

Fig. 5 Computed radial profiles of soot concentration

in the soot formation model⁽¹⁵⁾ and the soot combustion model⁽¹²⁾. This predicted soot concentrations are reasonable in comparison with the experimental results⁽¹⁶⁾ of a similar diffusion flame. It is assumed that the formation and combustion of soot are independent of the reactions of other species because the soot content in the combustion gas is smaller than that of combustion products.

The predicted maximum temperature tends to be higher than measured ones shown in Fig. 4(b), especially when the radiative heat transfer is ignored. By incorporating gaseous radiation first and soot radiation second, the predicted temperature profiles approach the experimental results stepwise and finally, fairly good prediction is obtained. By paying attention to the changes in temperature induced by the incorporation of radiative heat transfer, it is seen that the contribution of soot radiation is small in the maximum temperature region in the cross section of $L=50$ cm in spite of the relatively high content of soot. It is, however, nearly the same as the contribution of gaseous radiation. The contribution of soot radiation is much smaller than that of gaseous radiation in the circumferential and downstream regions where soot content is relatively low.

5.3 Effect of soot on heat flux at the furnace wall

Figures 6 and 7 show the axial profile of heat flux on the furnace wall computed without and with soot radiation, respectively, using the weighted-sum-of-gray-gas model. The broken line indicates the computed radiative heat flux to the wall except for the convective heat flux. The solid line shows the computed total heat flux including both radiative and convective contributions. The dots represent experi-

Fig. 6 Heat flux to the furnace wall computed with the weighted sum of the three gray-gas model without soot radiation

Fig. 7 Heat flux to the furnace wall computed with weighted sum of the three gray-gas model with soot radiation

mental data. It is worth noting that the contribution of convection heat transfer to the heat fluxes in the furnace wall is marginal as compared with the radiative heat transfer.

Figure 8 shows the distributions of radiative emission rate per unit volume. The broken line and the solid line correspond to Fig. 6 (without soot radiation) and Fig. 7 (with soot radiation), respectively.

The heat flux to walls in the upstream region increases by incorporating soot radiation, and corresponds to the increase in radiative emission rate shown in Fig. 8. In this region, the heat transfer by convection is small. The contribution of soot radiation

Fig. 8 Distributions of radiative emission rate per unit volume (broken line: without soot radiation, solid line: with soot radiation)

to the wall heat transfer is almost equal to that of gaseous radiation. However, the increase in the amount of heat accepted by the wall leads to an increased temperature drop in the upstream region, as shown in Fig. 4(a) and, as shown in Fig. 8, the radiative emission rate is suppressed for cross sections over $L=250$ cm because soot is hardly predicted in such regions (see Fig. 5). As a result, the wall heat flux decreases in the downstream region, and the total amount of heat given to the furnace wall does not increase, as noted from Figs. 6 and 7.

5.4 Comparison with exponential wide-band model

Figure 9 shows the axial profile of heat flux to the furnace wall computed using the exponential wide-band model⁽¹⁰⁾. The contribution of soot radiation is neglected in this case. Accordingly, these results correspond to those in Fig. 6. When radiative heat transfer to the furnace wall is computed using the exponential wide-band model, the entire wave number domain (from 0 to 8000 cm^{-1}) is divided into 800 subdomains. Considering that the absorption bands of CO_2 and H_2O pile up at $2.7\text{ }\mu\text{m}$, the absorption coefficient K is expressed as follows.

$$K\eta = k_{\text{CO}_2}(\eta)p_{\text{CO}_2} + k_{\text{H}_2\text{O}}(\eta)p_{\text{H}_2\text{O}}$$

Assuming that the respective mass absorption coefficients of CO_2 and H_2O is replaced with s/d (d : the interval of line spectrums, s : the intensity of line spectrum), $k_{\text{CO}_2}(\eta)$ and $k_{\text{H}_2\text{O}}(\eta)$ are converted to be the pressure absorption coefficients at band η . Here, p_{CO_2} and $p_{\text{H}_2\text{O}}$ are partial pressures of species in the combustion gas.

The weighted-sum-of-gray-gas model holds when

Fig. 9 Heat flux to the furnace wall computed using the exponential wide-band model without soot radiation

the spectral patterns of absorption coefficients vary similarly over an entire wave number domain with temperature variation. Real combustion gas, however, does not exhibit such an ideal characteristic. From the rigorous point of view, the weighted-sum-of-gray-gas model is unreasonable for application to nonisothermal problems such as furnace heat transfer. On the other hand, the comparison between Figs. 7 and 9 suggests that the weighted-sum-of-gray-gas model can be acknowledged as a practical calculation method, as long as it is used in the prediction of radiative heat flux to the furnace wall.

6. Summary

Numerical simulations of heat transfer in a furnace of practical scale were carried out, coupled with a prediction of the flame and the nongray characteristic of gaseous radiation into account. The results are summarized as follows.

(1) The profiles of temperature and species concentration can be predicted fairly well and are sufficiently available as the basis for the estimation of radiative and convective heat transfer in a wall.

(2) The weighted sum of three-gray-gas model gives a good prediction of heat flux to the furnace wall, which is almost same as the prediction using a wide-band model. The influence of soot on furnace heat transfer was also estimated.

(3) Though the heat flux on the furnace wall in the upstream region increases with considering soot radiation, it decreases in the downstream region. Consequently, the total amount of heat given to the furnace wall is almost the same even if soot radiation

is incorporated.

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