Application of WSGSA Model in Predicting Temperature and Soot in C_2H_4/Air Turbulent Diffusion Flame

HE Zhenzong[1], *ZHU Ruihan*[1], *DONG Chuanhui*[1], *MAO Junkui*[1*], *FU Yao*[2]

1. College of Energy and Power Engineering, Nanjing University of Aeronautics and Astronautics, Nanjing 210016, P. R. China;

2. Aviation Key Laboratory of Science and Technology on Aero Electromechanical System Integration, Nanjing 211106, P. R. China

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Abstract: Soot, a product of insufficient combustion, is usually in the form of aggregate. The multi-scattering of soot fractal aggregates has been proved to play an important role in studying the soot radiative properties, which is rarely considered in predicting the radiative heat transfer in combustion flame. In the present study, based on the weighted sum of gray soot fractal aggregate (WSGSA) model, which is used to predict the temperature field and soot aggregates in turbulent diffusion flame, the flame temperature distribution and soot volume fraction distribution under the conditions of the model without considering radiation, the default radiation model in Fluent software and the WSGSA model are calculated respectively. The results show that the flame temperature will be seriously overestimated without considering radiation and the maximum relative discrepancy of flame centerline temperature is about 64.5%. The accuracy will be improved by the default radiation model in the Fluent software, but the flame temperature is still overestimated and the maximum relative discrepancy of flame centerline temperature is about 42.1%. However, more satisfactory results can be obtained by the WSGSA model, and the maximum relative discrepancy of flame centerline temperature is no more than 15.3%. Similar conclusions can also be obtained in studying the temperature distribution along different flame heights. Moreover, the soot volume fraction can be predicted more accurately with the application of the WSGSA model. Both without considering radiation and using the default radiation model in the Fluent software will result in the underestimating of soot volume fraction. All the results reveal that the WSGSA model can be used to predict the temperature and soot aggregates in the C_2H_4/air turbulent diffusion flame.

Key words: radiative heat transfer; WSGSA model; soot radiation; turbulent diffusion flame; soot aggregate

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0 Introduction

Radiative heat transfer is critical to the research on combustion and heat transfer mechanisms of the combustion flame[1]. As the main product of insufficient combustion of hydrocarbon fuels, the soot can emit radiant energy strongly and continuously in the whole infrared spectrum[2], which has been proved to be the second largest factor of greenhouse effect and global warming, second only to carbon dioxide[3]. Experimental research proves that the ability of emitting radiant energy of soot is far stronger than that of participated gas at the same temperature[2]. Although the volume fraction of soot is small, the ability of emitting radiant energy cannot be ignored and the spectral radiant intensity of flame is mainly determined by the soot. Therefore, establishing an efficient and accurate calculation model to study the radiative properties of the soot and gas is of great significance for experimental design and pollutant

*Corresponding author, E-mail address: mjkpe@nuaa.edu.cn.

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emission control.

The radiative properties of high temperature gases strongly depend on parameters such as wave number, temperature and pressure, which bring great difficulties to solve the radiative transmission equation. Generally, the common numerical calculation models used to predict the radiative transfer in the gas medium include line-by-line (LBL) model, band model (BM) and global model (GM). The LBL model shows the highest calculation accuracy and the spectral variable information can be fully taken into account by integrating over all wave number intervals. However, this model usually needs a huge spectral database, which has the slowest calculation speed and high requirements for calculation resources, therefore, it cannot be applied to engineering calculation. The BM model considers both calculation efficiency and calculation accuracy. The main idea of BM model is replacing its spectral radiative characteristic parameters by the average value of radiative characteristic parameters in spectral integration interval. The GM model is an effective balance between calculation efficiency and calculation accuracy. In the actual process of radiative heat transfer calculations, we tend to care more about the total radiative heat flux and radiative source within the whole wave number. The GM model can integrate the radiative characteristic parameters in the whole spectral range and solve the radiative transfer equation only for very few times. Moreover, it can be combined with different methods for solving the radiative transmission equation and can be effectively coupled with computational fluid dynamics software. Generally, the GM model mainly includes Planck average absorption coefficient model, weighted-sum-of-gray-gases (WSGG) model, spectral-line-based WSGG (SLW-WSGG) model, full-spectrum k-distribution (FSK) model and various extended models based on these models. The WSGG model, first proposed in Ref.[4] in 1967, is widely used for its high efficiency, simplified calculation process and relatively high calculation accuracy. The model can be combined with any form of radiative heat transfer equation and it can realize the coupling solution of radiation, convection and heat conduction by embedding user-defined functions into computational fluid dynamics software, which makes the WSGG model develop rapidly. Through the continuous efforts of many scholars, from the initial model parameters only applicable to specific H_2O/CO_2 partial pressure ratio[5], a variety of WSGG model parameters applicable to different H_2O/CO_2 partial pressure ratios[6], oxygen-rich combustion[7-8] and high-pressure combustion[9] have been gradually developed. With the release of the latest molecular spectrum database HITEMP2010, many new WSGG model parameters obtained by fitting emissivity based on HITEMP2010 database have fully expanded the applicable temperature range and pressure range[10-11].

The soot produced by hydrocarbon fuel combustion usually exists in the form of fractal aggregate and the aggregate may contain hundreds of primary particles. The primary particle size range is generally between 10 nm and 60 nm, and may reach 300 nm in extreme cases. To accurately calculate the radiative properties of fractal aggregate of soot, many numerical calculation models have been developed, such as generalized multi-particle MIE theory (GMM) model[12], multi-sphere-T-matrix (MSTM) [13] and method of moment(MOM), etc. The approximate models include Rayleigh-Deybe-Gans-fractal-aggregate (RDG-FA) model, discrete Diople approximation (DDA), finite difference time domain (FDTD), and the equivalent-sphere model.

Recently, considerable work has reported the studies of the radiative heat transfer in the gas and soot mixture[7-8]. The soot is usually assumed to be single and dispersed, and the effect of soot aggregation is rarely considered. In fact, the soot aggregation has been proved to affect the radiative properties of soots obviously. In Refs.[1, 14], the influences of soot aggregation on the radiative heat transfer in homogeneous gas-soot mixtures were also studied on the basis of the FSK model and GMM theory, and the results revealed that ignoring the ef-

fect of soot aggregation would overpredict the radiative heat transfer properties of the mixture. Therefore, to predict the radiative heat transfer in the gas-soot mixture including aggregates more accurately, the effect of soot fractal aggregation should be considered. Therefore, a model, named weighted sum of gray soot fractal aggregate (WSGSA) model, is developed by combining the features of the FSK model with WSGG model. More details can be achieved in Refs. [1, 14]. By using the WSGSA model the heat transfer properties of the C_2H_4/air turbulent diffusion flame are studied in the present work. The flame temperature distribution and soot volume fraction distribution are calculated respectively under the conditions of the model without considering radiation, the default radiation model in Fluent software and the WSGSA model. Finally, the accuracy of the WSGSA model is verified by combined with the WSGG model in the Fluent software.

1 Physical Model

In this paper, the coaxial C_2H_4 /air turbulent diffusion flame experiment carried out by Kent et al.[15] is taken as the research object. As a classic experiment measuring the axial temperature distribution, radial temperature distribution and soot volume fraction distribution, it has been used as the benchmark to verify the numerical calculation results for many times in the past decades[16-17]. The calculation domain model is shown in Fig.1. The fuel preheated to 322 K (pure C_2H_4) is shot into the air at an average speed of 52 m/s through a nozzle with an inner diameter of 3.0 mm to form a diffusion flame. The Reynolds number at the nozzle outlet is Re=14 660. Since the flame has two-dimensional axisymmetric characteristics, half of the calculation domain is taken for non-uniform mesh division to improve the calculation efficiency. Moreover, the mesh encryption is carried out for the fuel nozzle outlet and the area near the axis of symmetry. The mesh division results are shown in Fig.2, where r represents the radius and Z the direction of the flow.

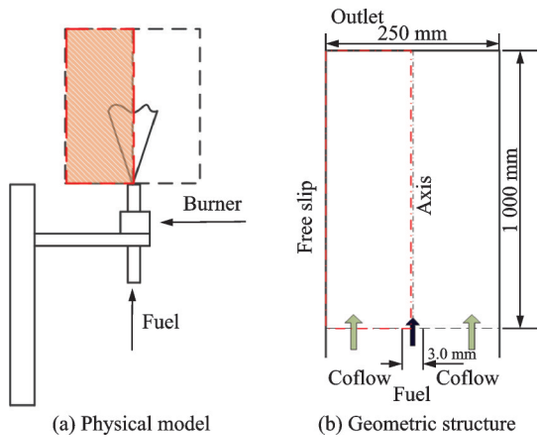


Fig.1 Physical model and geometric structure diagram of research object[14]

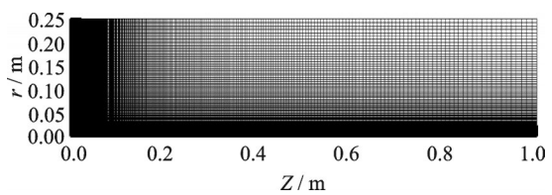


Fig.2 Non-uniform grid division diagram in computational domain

2 Computational Model

2.1 Governing equation

The standard k-ε turbulence model is adopted. The transport equations of mass conservation, momentum conservation, energy conservation, turbulent kinetic energy and turbulent kinetic energy dissipation rate can all be given in the general form of Eq.(1).

$$\frac{\partial \rho\phi}{\partial t}+\frac{\partial}{\partial x_i}(\rho u_i\phi)-\frac{\partial}{\partial x_i}\left(\Gamma_\phi\frac{\partial \phi}{\partial x_i}\right)=S_\phi \quad (1)$$

where ρ, t, ϕ, Γ_ϕ and S_ϕ denote the density, the time, the scalar, the diffusion coefficient and the source term, respectively, which are summarized in Table 1, where μ represents the velocity of the component , Pr the Planck number, ε the emissivity, σ the spectral scattering coefficient, and f the fraction of the mixture.

2.2 Combustion model

The combustion model in this paper is a steady laminar flame surface model, and the turbulent flame can be regarded as a set of one-dimensional laminar structures. To express the flame by

Table 1 Corresponding scalar, diffusion coefficient and source term in governing equations

Equation	ϕ	Γ_ϕ	S_ϕ
Mass conservation	1	0	0
Momentum conservation	u_i	$\mu+\mu_t$	$-\frac{\partial}{\partial x_j}\left(p+\frac{2}{3}\rho k+\frac{2}{3}(\mu+\mu_t)\frac{\partial u_i}{\partial x_i}\right)+\frac{\partial}{\partial x_i}\left[(\mu+\mu_t)\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)\right]$
Energy conservation	h	$\frac{\mu}{Pr}+\frac{\mu_t}{Pr_t}$	$\nabla\cdot q$
Turbulence kinetic energy	k	$\mu+\frac{\mu_t}{\sigma_k}$	$G_k-\rho\varepsilon$
Turbulent kinetic energy dissipation rate	ε	$\mu+\frac{\mu_t}{\sigma_\varepsilon}$	$\frac{\varepsilon}{k}(C_{1\varepsilon}G_k-C_{2\varepsilon}\rho\varepsilon)$
Mixture fraction	$\bar{f}$	$\frac{\mu+\mu_t}{\sigma_t}$	0
Mixture fractional pulsation	$\overline{f'^2}$	$\frac{\mu+\mu_t}{\sigma_t}$	$C_g\mu_t\left(\frac{\partial\bar{f}}{\partial x_j}\right)^2-C_d\bar{\rho}\frac{\varepsilon}{k}\overline{f'^2}$
C	c	$\frac{\mu_t}{S_{c_t}}$	ρS_c

the isosurface of mixed components, the left and right components are assumed to behave the same diffusion coefficient. The coefficient values of σ_t, C_g and C_d are set as 0.85, 2.96 and 2.0, respectively. The premixed combustion is modeled by C equation model and the reaction process is represented by scalar C. The transport equation of scalar C is shown in Table 1. The value range of scalar C is set as [0, 1], where 0 represents unburned reactant and 1 represents burnt reactant. The effects of turbulent pulsation on flame temperature, composition and density are established by using probability density function (PDF). The GRI3.0 detailed chemical reaction mechanism[18] is adopted.

2.3 Soot generation model

The Moss-Brookes two-equation model in the semi-empirical model is used to predict the soot generation. The model obtains the soot volume fraction distribution by solving the transport equation of soot nucleation aggregation and soot mass fraction[19]

$$\frac{\partial}{\partial t}(\rho Y_{soot})+\nabla\cdot(\rho\boldsymbol{v}_{soot})=\nabla\cdot\left(\frac{\mu_t}{\sigma_{soot}}\nabla Y_{soot}\right)+\frac{dM}{dt} \tag{2}$$

$$\frac{\partial}{\partial t}(\rho b^*_{nuc})+\nabla\cdot(\rho\boldsymbol{v}b^*_{nuc})=\nabla\cdot\left(\frac{\mu_t}{\sigma_{nuc}}\nabla b^*_{nuc}\right)+\frac{1}{N_{norm}}\frac{dN}{dt} \tag{3}$$

where Y_{soot} represents the soot mass fraction, M the soot nucleation aggregation, $N_{norm}=10^{15}$, b^*_{nuc} the normalized atoms nucleation concentration ($b^*_{nuc}=N/\rho N_{norm}$), μ_t/σ_{soot} the diffusion coefficient of soot mass fraction, and μ_t/σ_{nuc} the diffusion coefficient of atom nucleation concentration.

It is assumed that C_2H_2 and C_2H_4 are the chemical components of soot nucleation, surface growth and other chemical reactions. The oxidation model is Lee model, in which hydroxyl [OH] is used as the oxidant and the concentration of locally balanced hydroxyl [OH] and equilibrium oxygen atom [O] can be respectively expressed by

$$[OH]=2.129\times10^2T-0.57e^{-4\,595/T}[O]^{1/2}[H_2O]^{1/2} \tag{4}$$

$$[O]=3.97\times105T^{-1/2}e^{31\,090/T}[O_2]^{-1/2} \tag{5}$$

2.4 Radiation model

2.4.1 Radiative transfer equation

For a one-dimensional dispersive mixed medium with absorption, emission and scattering properties composed of participating gases (such as H_2O, CO_2, etc.) and soot, the internal spectral radiative transfer process can be described by the one-dimensional spectral radiative transfer equation[19]

$$\frac{\partial I_\lambda(z,\boldsymbol{s})}{\partial s}=\kappa_{\mathrm{m},\lambda}I_{\mathrm{b},\lambda}(T_\mathrm{m},z)-\kappa_{\mathrm{m},\lambda}I_\lambda(z,\boldsymbol{s})-\sigma_{\mathrm{m},\lambda}I_\lambda(z,\boldsymbol{s})+\frac{\sigma_{m,\lambda}}{4\pi}\int_{4\pi}I_\lambda(z,\boldsymbol{s})\Phi(\boldsymbol{s},\boldsymbol{s})\mathrm{d}\Omega' \quad (6)$$

where $I_\lambda(z,\boldsymbol{s})$ is the spectral radiation intensity in the direction at position z, $I_{\mathrm{b},\lambda}(T_\mathrm{m},z)$ the blackbody spectral radiation intensity at position z and the temperature T_m, $\Phi(\boldsymbol{s},\boldsymbol{s})$ the scattering phase function of the mixed medium, Ω' the solid angle, and $\kappa_{\mathrm{m},\lambda}$ the spectral absorption coefficient in the mixed medium. $\kappa_{\mathrm{m},\lambda}=\kappa_{\mathrm{gas},\lambda}+\kappa_{\mathrm{soot},\lambda}$, $\kappa_{\mathrm{gas},\lambda}$ and $\kappa_{\mathrm{soot},\lambda}$ represent the spectral absorption coefficients of the participating gas and soot respectively. $\sigma_{\mathrm{m},\lambda}$ represents the spectral scattering coefficient of the mixed medium. The boundary condition of non-grey boundary is[20]

$$I_\lambda(z_\mathrm{w},\boldsymbol{s})=\varepsilon_\mathrm{w}I_{\mathrm{b},\lambda}(T_\mathrm{w},z_\mathrm{w})+\frac{1-\varepsilon_\mathrm{w}}{\pi}\int_{\boldsymbol{sn}<0}I_\lambda(z_\mathrm{w},\boldsymbol{s})|\boldsymbol{s},\boldsymbol{n}|\mathrm{d}\Omega \quad (7)$$

where ε_w is the wall emissivity, $\varepsilon_\mathrm{w}=1$ the blackbody wall, $I_{\mathrm{b},\lambda}$ the blackbody spectral radiation intensity at the wave number λ, T_w the temperature of the wall, and $\boldsymbol{n}$ the outer normal direction vector of the wall. z_w and $\boldsymbol{s}$ are the location coordinates.

According to the WSGG model theory, soot can also be regarded as non-gray medium, just like participating gases. Therefore, the radiative transfer equation and boundary conditions in the mixed medium containing participating gas and soot can be written as follows[21]

$$\sum_{i=1}^{N}\frac{\mathrm{d}I_{\mathrm{m},i}(z,\boldsymbol{s})}{\mathrm{d}\boldsymbol{s}}=\sum_{i=1}^{N}\kappa_{\mathrm{m},i}I_\mathrm{b}(T_\mathrm{m},z)a_{\mathrm{m},i}(T_\mathrm{m})-\sum_{i=1}^{N}\kappa_{\mathrm{m},i}I_{\mathrm{m},i}(z,\boldsymbol{s})-\sum_{i=1}^{N}\sigma_{\mathrm{m},i}I_{\mathrm{m},i}(z,\boldsymbol{s})+\sum_{i=1}^{N}\frac{\sigma_{\mathrm{m},i}}{4\pi}\int_{4\pi}I_{\mathrm{m},i}(z,\boldsymbol{s})\Phi(\boldsymbol{s},\boldsymbol{s})\mathrm{d}\Omega' \quad (8)$$

$$\sum_{i=1}^{N}I_{\mathrm{m},i}(z_\mathrm{w},\boldsymbol{s})=\sum_{i=1}^{N}\varepsilon_{\mathrm{m},i}I_\mathrm{b}(T_\mathrm{w},z_\mathrm{w})a_{\mathrm{m},i}(T_\mathrm{w})+\sum_{i=1}^{N}\frac{1-\varepsilon_{\mathrm{m},i}}{\pi}\int_{4\pi}I_{\mathrm{m},i}(z_\mathrm{w},\boldsymbol{s})|\boldsymbol{s}\cdot\boldsymbol{n}|\mathrm{d}\Omega' \quad (9)$$

where N represents the number of grey medium selected, ε the emitting rate of the boundary, and $\kappa_{\mathrm{m},i}$ the absorption coefficient of the ith gray mixture consisting of gas and soot fractal aggregates. $\kappa_{\mathrm{m},i}=\kappa_{\mathrm{gas},i}+\kappa_{\mathrm{soot},i}$, $\kappa_{\mathrm{gas},i}$ and $\kappa_{\mathrm{soot},i}$ represent the spectral absorption coefficients of the ith participating gas and soot, respectively. $\sigma_{\mathrm{m},i}$ represents the spectral scattering coefficient of the ith gray mixture consisting of gas and soot fractal aggregates. $a_{\mathrm{m},i}(T_\mathrm{m})$ represents the weight factor of the ith gray mixture consisting of gas and soot fractal aggregates at the Gaussian integral point, $a_{\mathrm{m},i}(T_\mathrm{m})=a_{\mathrm{gas},i}(T_\mathrm{m})\times a_{\mathrm{soot},i}(T_\mathrm{m})$. $a_{\mathrm{gas},i}(T_\mathrm{m})$ represents the weighting factor of the ith gray gas, and $a_{\mathrm{soot},i}(T_\mathrm{m})$ the weighting factor of the ith soot. In this paper, the discrete ordinates model of Fluent software platform is used to solve the radiative transfer equation, in which the gas radiation model and the soot radiation model are described below.

2.4.2 Gas emission model—WSGG

The common participating gases in combustion products include H_2O and CO_2. According to the WSGG model theory, the absorption coefficient of the ith gray gas and the corresponding weight factor can be obtained by fitting the calculation results of the LBL model. Therefore, the emissivity ε_gas in the pure participatory gas medium can be expressed as[19]

$$\varepsilon_\mathrm{gas}(T)=\sum_{i=1}^{N_\mathrm{gas}}a_{\mathrm{gas},\mathrm{g}_i}(T)\left\{1-\exp\left[-\kappa_{\mathrm{gas},\mathrm{g}_i}P_\mathrm{gas}L\right]\right\} \quad (10)$$

where N_gas represents the number of non-gray gases selected, $a_{\mathrm{gas},\mathrm{g}_i}(T)$ the weight factor related to temperature, P_gas the partial pressure of gas, T the gas temperature, and L the thickness of the medium.

2.4.3 Soot aggregates radiation model—WSGSA

Based on the WSGG model and the basic idea of full spectral k distribution, the spectral radiative properties of soot aggregates, e.g. absorption cross section and scattering cross section, are predicted by the RDG-FA model for different arrangements at first. Then, these spectral radiative properties are reordered in smoothly-varying g-space according the principle of FSK model, and the values at the Gaussian-Legendre quadrature integral points in the g-space are obtained. Finally, according to principle of the WSGG model, the relationship between the radiative properties at the Gaussian-Legendre quadrature integral points and the geometric characteristic parameters of the soot aggregates, e.g. pri-

mary particle number, are obtained by data fitting.

The cluster-cluster aggregation (CCA) model, developed by Mackowski et al.[13] and widely used in studying the aggregation of soot and aerosols, is proposed to study the soot aggregation process in the present work. The details of the CCA model is available in Refs.[1,14]. According to the fractal theory, the morphology and construction of the aggregate can be described as

$$N_s = k_f\left(\frac{2R_g}{d_p}\right)^{D_f} \tag{11}$$

$$R_g^2 = \frac{1}{N_s}\sum_{i=1}^{N_s} r_i^2 \tag{12}$$

where N_s is the total number of the primary monomers in the aggregate, d_p the mean diameter of the monomers, k_f the fractal prefactor, D_f the fractal dimension, R_g the root mean square radius that quantifies the overall size of the aggregate and is called the gyration radius, and r_i the distance from the ith sphere to the center of the aggregate mass. The relationship between the gyration radius R_g and the number of monomers N_s in the aggregates can thus be connected by the fractal dimension D_f and fractal prefactor k_f.

According to Refs.[1,14], the values for the fractal dimension D_f of the soot fractal aggregates almost fall within the range of 1.6—1.9, the particle size of the soot is set as 33 nm to simplify the calculation process and make the problem mathematically trackable, and the total number of the primary monomers in the soot fractal aggregates is set in the range of 20—300.

$$\varepsilon_{soot}(T) = \sum_{j=1}^{N_{soot}} a_{soot,g_j}(T)\left\{1-\exp\left[-\kappa_{soot,g_j}L\right]\right\} \tag{13}$$

where N_{soot} represents the number of gray soot aggregates selected, T the gas temperature, L the thickness of the medium, and $a_{soot,g_j}(T)$ the weight factor related to temperature, which can be expressed as

$$a_{soot,g_j}(T) = \sum_{i=1}^{I} c_{soot,g_j,i}\,T^{i-1} \tag{14}$$

where $c_{soot,g_j,i}$ represents the i-order polynomial coefficient of the jth soot aggregates, and a_{soot,g_j} the absorption coefficient of the jth soot aggregates in the dispersion medium

$$\kappa_{abs,j} = \sum_{i=1}^{n} C_{abs,j,N_{s,i}}^{agg}\frac{f_{v,i}}{N_{s,i}\pi d_p^3/6} \tag{15}$$

where $f_{v,i}$ represents the aggregate volume concentration of soot, and $N_{s,i}$ the number of particles in the aggregate of soot. In addition, the scattering phase function Henyey-Greenstein(H-G) of soot aggregates can be expressed as

$$\Phi_{g_j}(\boldsymbol{s},\boldsymbol{s}) = \frac{1}{\sigma_{soot,g_j}}\sum_{i=1}^{n} C_{sca,g_j,N_{s,j}}^{agg}\cdot \frac{f_{v,i}}{N_{s,i}\pi d_p^3/6}\Phi_{g_j,N_{s,i}}(\boldsymbol{s},\boldsymbol{s}) \tag{16}$$

$$\Phi_{g_j,N_{s,i}}(\boldsymbol{s},\boldsymbol{s}) = \frac{1-(g_{0,g_j,N_{s,i}}^{agg})^2}{\left[1+(g_{0,g_j,N_{s,i}}^{agg})^2-2g_{0,g_j,N_{s,i}}^{agg}\cos(\boldsymbol{s},\boldsymbol{s})\right]^{1.5}} \tag{17}$$

where $g_{0,g_j,N_{s,i}}^{agg}$ represents the asymmetry factor of soot aggregates.

According to the previous research results of our team, the radiative properties of soot aggregates are correlated with the number of soot monomers in the aggregates[22-25], and the absorption coefficient is linearly correlated with the number of particles in the aggregate. Therefore, the absorption coefficient of soot aggregates C_{abs,g_j,N_s}^{agg} can be expressed as

$$C_{abs,g_j,N_s}^{agg} = p_j N_s + p_{0,j} \quad N_s\in[20,300] \tag{18}$$

where p_j and $p_{0,j}$ represent the polynomial coefficients of the jth soot aggregate. Different from the absorption coefficient, the aggregate scattering coefficient C_{sca,g_j,N_s}^{agg}, asymmetry factor g_{0,g_j,N_s}^{agg} and the number of monomer particles in soot meet multiple power correlation are

$$C_{sca,g_j,N_s}^{agg} = \sum_{i=1}^{m} q_{j,i}N_s^{m-i} \quad N_s\in[20,300] \tag{19}$$

$$g_{0,g_j,N_s}^{agg} = \sum_{i=1}^{m} o_{j,i}N_s^{m-i} \quad N_s\in[20,300] \tag{20}$$

where $p_{0,j}$, $q_{j,i}$ and $o_{j,i}$ can be obtained through data fitting. For detailed research process, please refer to Ref.[1].

2.5 Default model in Fluent software

In this paper, the high-temperature gas absorption coefficient model and soot absorption coefficient model in the Fluent software are used to verify the WSGSA model, which is recorded as the de-

fault model. The high-temperature gas radiation model in the Fluent software is based on the WSGG model developed by Smith in 1982[14], and the total absorption coefficient is calculated by calculating the total emissivity

$$\kappa_g = -\frac{\ln(1-\varepsilon)}{S} \tag{21}$$

where $S=3.6V/A$ is the optical thickness, V the total volume of the calculation domain, and A the total surface area of the calculation domain.

The default soot absorption coefficient model in the Fluent software is

$$\kappa_s = b_1 \rho_{soot} Y_{soot}[1 + b_T(T-2\,000)] \tag{22}$$

where $b_1=1\,231.4$ m^2/kg, $b_T=4.8e^{-4}$ K^{-1}.ρ_{soot} and Y_{soot} are the density and mass fraction of soot aggregate.

So, the absorption coefficient of the gas-soot mixture can be expressed as

$$\kappa_{g,s} = \kappa_g + \kappa_s \tag{23}$$

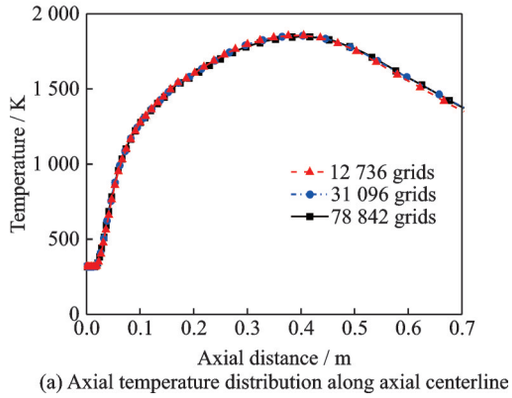
where κ_g and κ_g are the absorption coefficients of the gas and the soot, respectively.

3 Simulation Results and Discussion

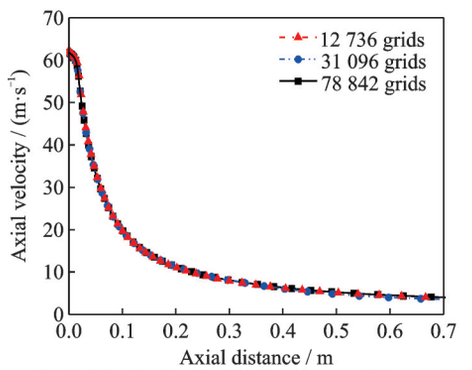
The flame temperature distribution and soot volume fraction distribution under the condition of the model without considering radiation, the default radiation model in Fluent software and the WSGSA model are calculated respectively in the coaxial C_2H_4/air turbulent diffusion flame.

3.1 Grid independence validation

To verify that the calculated results are independent of the number of grids, this section carries out numerical calculations with three sets of grids with the number of 12 736, 31 096 and 78 842, respectively. The obtained axial velocity and temperature distributions along the axis of symmetry are shown in Figs.3(a) and (b), respectively. It is clear that there is a slight difference in temperature between the 12 736 grids and the other two sets of grids and there is almost no difference between the results of 31 096 grids and 78 842 grids. To increase the computational efficiency, 31 096 grids are used for subsequent research.



(a) Axial temperature distribution along axial centerline



(b) Axial velocity distribution along axial centerline

Fig.3 Grid independence verification

3.2 Results analysis

Fig.4 shows the flame centerline temperature compared with the experimental values. It can be seen that the prediction values of the WSGSA model developed in this paper are in good agreement with the experimental values and the maximum relative discrepancy is no more than 15.3%. When the axial distance is within 0.17 m, all the three models have a good agreement with the experimental values. However, when the axial distance exceeds 0.17 m, the flame temperature will be seriously overestimated without considering radiation, the maximum temperature will reach 2 191 K, which is 585 K away from the experimental values and the maximum relative discrepancy reaches 64.5%. The default model in the Fluent software and WSGSA model has almost the same prediction values when the axial distance is within 0.33 m, but the prediction values will also be overestimated by the default model when the axial distance exceeds 0.33 m, and the maximum relative discrepancy against the experimental values is about 42.1%, which is better than that without considering radiation.

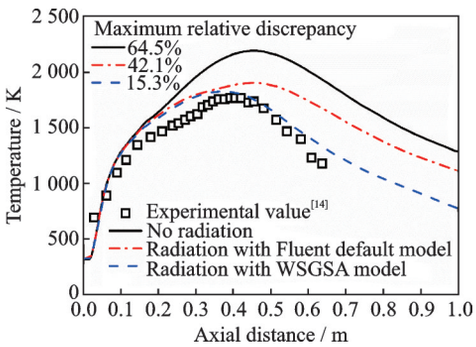


Fig.4 Axial temperature distribution of flame center line

Figs.5(a,b,c) are the temperature distribution cloud without considering radiation, calculated by the default model in the Fluent software, and obtained by the WSGSA model, respectively.

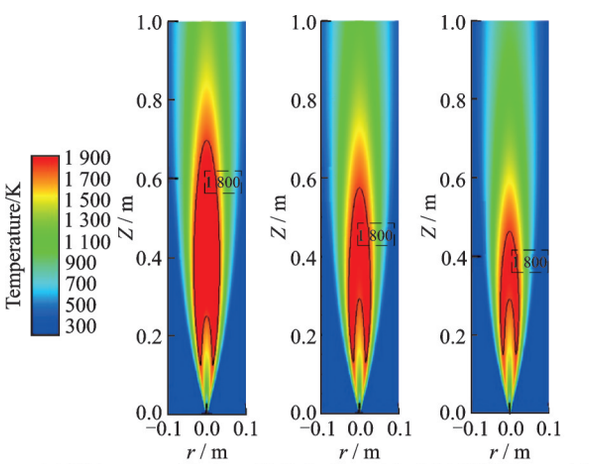


Fig.5 Temperature distribution cloud under different radiation model conditions

The solid black line is an isothermal line with a temperature equal to 1 800 K and the temperature surrounded by the solid black line is more than 1 800 K. It can be seen that when radiation is not considered, the high temperature range is the largest, followed by the Fluent software default model and the high temperature range is the smallest by WSGSA model. So, it is obvious that when radiation is not considered, not only the flame temperature will be overestimated, but the high temperature range of the flame will also be overestimated.

Similar conclusions can be obtained from the radial flame temperature distribution at different flame height positions. Fig.6 shows the radial flame temperature distribution at flame height Z=0.138, 0.241 5, 0.345 m, respectively. It can be seen from Fig.6 that the prediction radial flame temperature distribution by WSGSA model has the best agreement with the experiment values at different flame height positions. When radiation is not considered, the radial flame temperature will be overestimated at all heights, especially at flame height Z=0.345 m. The predicton values of the default model are better than the model which does not consider radiation but are worse than WSGSA model.

Fig.7 shows the radial soot volume fraction distribution at the flame heights Z=0.138, 0.241 5, 0.345 m, respectively. The soot volume fraction predicted by WSGSA model is in good agreement with the experimental value. Especially at Z=

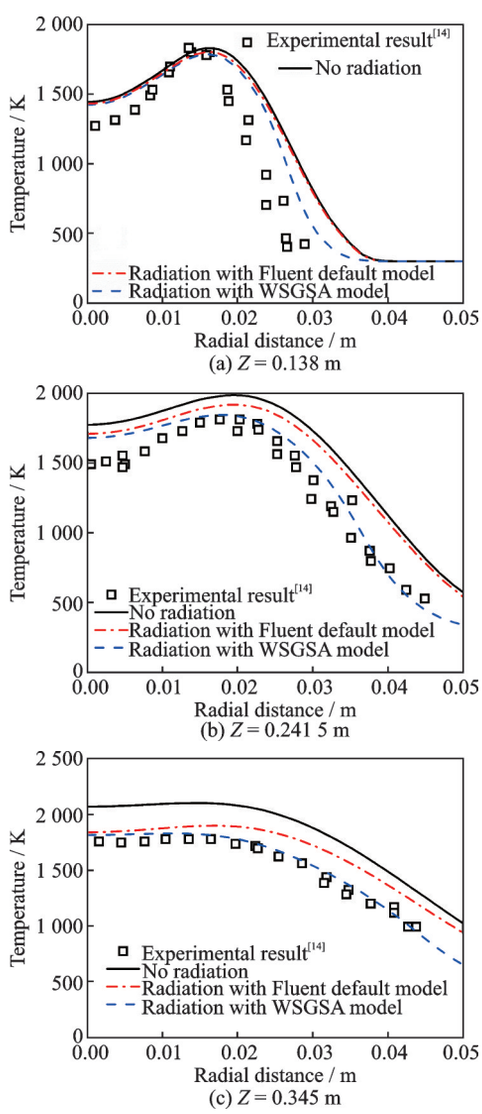


Fig.6 Radial temperature distribution at different flame heights

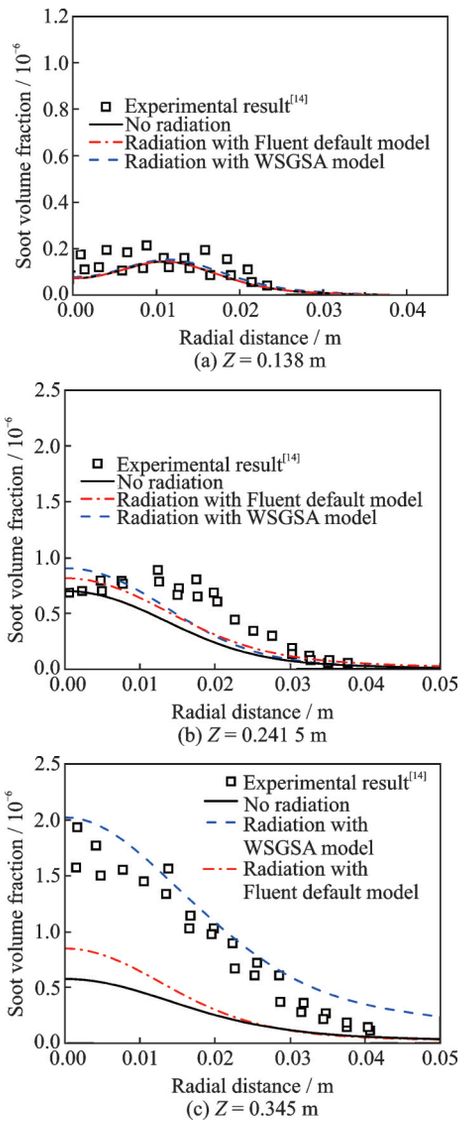


Fig.7 Radial soot concentration distribution at different flame heights

0.345 m, the maximum relative error is no more than 30%, which is more accurate than the results obtained without considering the radiative heat transfer or using the radiation with Fluent default model. The soot volume fraction will be underestimated in the other cases, especially without considering the radiation. The likely explanation may be that radiative heat transfer properties of soot can be accurately described by the WSGSA model, so more satisfactory flame temperature distribution can be obtained. As far as we know, the soot volume fraction is closely related to the flame temperature and the high temperature will enhance soot oxidation. Therefore, the soot volume fraction predicted by the WSGSA model is more satisfactory for more accurate temperature obtained.

4 Conclusions

The WSGSA model is used to predict the temperature distribution and soot volume fraction in the coaxial C_2H_4 /air turbulent diffusion flame. The results show that WSGSA model can not only be coupled with WSGG model and embedded in Fluent software platform, but also can more accurately predict the temperature distribution and soot concentration distribution of the flame, compared with cases without considering radiative heat transfer or with default model in Fluent software. The conclusions drawn from the results are as follows:

(1) The results reveal that the flame temperature will be seriously overestimated without considering radiation and the maximum relative discrepancy of flame centerline temperature is about 64.5%. The accuracy will be improved by the default radiation model in the Fluent software, but the flame temperature is still overestimated and the maximum relative discrepancy of flame centerline temperature is about 42.1%. However, more satisfactory results can be obtained by the WSGSA model, and the maximum relative discrepancy of flame centerline temperature is no more than 15.3%.

(2) The high temperature region will be reduced obviously with using the WSGSA model considered, which is conducive to decline the thermal protection requirements in an actual combustion device.

(3) The soot concentration distribution will be predicted more accurately with considering the radiative heat transfer, especially the WSGSA model being used.

The WSGSA model shows a good performance in predicting the temperature field and soot volume fraction of flame, which can be further applied to the prediction of the temperature and soot in the carbon and hydrogen flame soot.

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Authors Dr. **HE Zhenzong** received his Ph.D. degree in engineering thermophysics from Harbin Institute of Technology in 2016. He is currently an associate professor in Nanjing University of Aeronautics and Astronautics(NUAA). His research is focused on the radiative heat transfer of high gas and soot in the aero-engine combustion chamber, soot size inversion prediction and fuel cell system.

Prof. **MAO Junkui** received his Ph.D. degree in engineering from NUAA in 2003. He is currently a full professor in College of Energy and Power Engineering at NUAA. His research is focused on the aero-engine thermal management and efficient cooling technology and thermal analysis of aero-engine air system.

Author contributions Dr. **HE Zhenzong** contributed to the design of the study and wrote the manuscript. Prof. **MAO Junkui** contributed to the background and discussion and analysis of the study. Mr. **DONG Chuanhui** contributed to the discussion and analysis as well as prepared all drafts, and draw all the figures. Mr. **ZHU Ruihan** and Mr. **FU Yao** contributed to the discussion and analysis. All authors commented on the manuscript draft and approved the submission.

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WSGSA模型在C_2H_4/空气湍流扩散火焰温度和烟尘预测中的应用

贺振宗[1], 朱瑞韩[1], 董川徽[1], 毛军逵[1], 付　尧[2]

(1.南京航空航天大学能源与动力学院,南京 210016,中国;2.航空机电系统综合航空科技重点实验室,南京 211106,中国)

摘要:碳黑颗粒是燃烧不足的产物,通常以聚集体的形式存在。碳黑分形聚集体的多次散射特性已被证明在研究烟灰辐射特性方面起着重要作用,但在预测燃烧火焰中的辐射传热时很少考虑这一点。本文基于用于预测湍流扩散火焰中温度场和碳黑聚集体的灰体分形聚集体加权和(Weighted sum of gray soot fractal aggregate, WSGSA)模型,分别计算了模型不考虑辐射、Fluent软件默认辐射模型和WSGSA模型条件下的火焰温度分布和烟尘体积分数分布。结果表明,不考虑辐射会较大程度地高估火焰温度,火焰中心线温度的最大相对偏差约为64.5%。Fluent软件中的默认辐射模型将提高精度,但火焰温度仍然偏高,火焰中心线温度的最大相对偏差约为42.1%。然而,WSGSA模型获得的结果更加精确,火焰中心线温度的最大相对偏差不超过15.3%。在研究沿不同火焰高度的温度分布时也可以得到类似的结论。此外,应用WSGSA模型还可以更准确地预测烟尘体积分数。不考虑辐射以及使用Fluent软件中默认的辐射模型都会导致碳黑体积分数偏低。所有结果显示,WSGSA模型可用于有效预测C_2H_4/空气湍流扩散火焰中的温度和碳黑聚集体分布。

关键词:辐射换热;WSGSA模型;烟尘辐射;火焰的湍流扩散;烟灰集料