Simulation of Turbulent Combustion in a Large Pulverized Coal Boiler Based on Turbulent Radiation Interaction and the Modified Soot Model

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ABSTRACT: A combustion heat transfer model suitable for engineering combustion simulation was developed. Using the model, pulverized coal combustion and the soot generation process were simulated in a 300 MW tangentially fired pulverized coal furnace. Here, we proposed a soot evolution model which includes the nucleation, growth, agglomeration, and oxidation processes in the pulverized coal combustion process based on the population balance method. In the process of heat transfer, the absorption coefficient is refined by considering the coal particles and soot radiation. Furthermore, turbulent radiation interaction (TRI) was introduced to the combustion model. Then, pulverized coal combustion and soot and NOX generation processes in a 300 MW tangentially fired pulverized coal furnace under different loads were studied. The results show that the simulated temperature field considering the effect of TRI is lower than that without TRI, and the simulation results considering the effect of TRI are closer to results from the field test. The error between the simulation results and the field tests is within 0.56%. The soot fraction is negatively correlated with temperature. The higher the temperature, the smaller the soot fraction. Taking into account the impact of TRI, the predicted soot production increased.

INTRODUCTION

Coal-fired power plants are the mainstay of electricity generation in China today. Soot generated during coal power generation is one of the particulate pollutants. It can seriously affect the environment and human health.

Soot radiation heat transfer and soot generation are strongly coupled and interact with each other. The soot has a great influence on the energy exchange of radiation during the combustion process. Lau and Niksa research shows that the radiant flux brought by soot plays an important role in coal combustion. Moreover, the volume fraction of soot generated by combustion, together with the temperature, is the key parameter that determines the radiative heat transfer in the furnace. If the generation of soot is ignored in the simulated combustion process, the flame temperature will be significantly different. Therefore, in order to reduce pollution and improve combustion efficiency, it is necessary to study the generation mechanism of soot and its effect on radiant heat transfer in the combustion process.

The production of soot is the result of soot formation, oxidation, and transportation. The formation mechanism of soot in turbulent combustion simulation mainly includes empirical models, semi-empirical models, detailed models, and so forth. The detailed model involves many complex chemical reaction processes. For coal combustion, it is a very complex process. A population balance model (PBM) can be used to construct a particle number density balance equation to solve for soot production, number density, and particle diameter. Then, the processes of soot nucleation, growth, agglomeration, and oxidation can be expressed. Among them, nucleation is an important initial stage of the soot generation process. The definition of the nucleation precursor is accurate or not reflects the accuracy of the model.

Considering its role, turbulent radiation interaction (TRI) can improve the computational accuracy of soot formation models. Many soot formation modeling studies have coupled radiation models, but most of them have used simpler models, such as the gray medium or optically thin approximation. Average temperature and average component concentrations were also applied to calculate the radiative source term and associated radiative properties, regardless of the influence of fluctuations. Such a processing method is sufficiently accurate in the radiation calculation of the nonreactive flow because the
scalar pulsation of the nonreactive flow is much smaller than the pulsation in flames. However, in actual turbulent combustion, turbulent pulsation will cause temperature and component pulsation, which will affect the related radiation field pulsation. This problem of affecting the interaction between turbulent pulsation on radiation intensity and radiation source pulsation is TRI. Therefore, this only stresses out the necessity to consider TRI to simulate soot generation. This is also supported by relevant studies. Mehta et al. found that for a given temperature, species and soot distribution, taking into account that TRI will increase emissions by 30–60%, and the net heat loss of flames will increase by 45–90%. This is due to radiant heat loss caused by TRI. Madejski et al. numerically simulated the pulverized coal combustion process of a swirling pulverized coal-fired boiler and also verified the effect of soot on radiative heat transferred.

For the numerical solution to the radiation equation for turbulent coal combustion processes, the application of DNS and stochastic methods can include TRI effects but at the high computational cost for practical engineering simulation. Therefore, for the calculation of the radiative heat transfer equation (RTE) for pulverized coal combustion, Reynolds average Navi-stokes (RANS) is the choice for engineering applications. The time-averaged RTE removes the effects of component fluctuations and temperature fluctuations. In order to solve the RTE using time averaging, while taking into account the role of TRI, the following three issues must be addressed. The first is the RTE equation itself; common methods are the spherical harmonics method, the discrete ordinates method (DOM), the finite volume method, the Monte Carlo method, and so on. DOM models are easily extended to higher orders, so they are commonly used for industrial burner calculations. The second is the calculation of gas radiation characteristic parameters, which have correlated the k-distribution method or global models (weighted sum of gray gases (WSGG), spectral line-based weighted sum of gray gases, full-spectrum k-distribution, etc.). Considering the calculation difficulty and calculation accuracy, the WSGG model is a better choice. Moreover, for the numerical simulation of pulverized coal combustion radiation, the calculation of the radiation parameters of particles and soot should not be ignored. The third is TRI solution. There are many ways to solve TRI, such as solving the pulsation value of a turbulent scalar using stochastic methods, which require large computational resources. There is direct solving of TRI based on LES. The amount of computation is also large. Therefore the scalar joint PDF and time-averaged RTE coupling are a better way to solve TRI.

Based on the RANS-PBM-PDF model, this paper establishes a model that can accurately describe the turbulent combustion of pulverized coal and the generation of soot. Nucleation, growth, agglomeration, and oxidation processes of soot are considered to construct a PBM that accurately describes soot generation. Refinement of the RTE model for coal combustion is carried out by considering gas and particulate radiation. A scalar joint PDF was used to calculate the component and temperature pulsations, which was combined with the RTE model to calculate TRI. The distribution characteristics of CO, NO, SO, and O in a 300 MW pulverized coal boiler under different working conditions are simulated. Compare the difference in temperature, soot generation, and NO emissions in the furnace with and without TRI. This article provides a more accurate mathematical model of combustion. It can better describe the nucleation, growth, agglomeration, and oxidation processes of soot. Combining turbulent pulse action with radiation will help to understand the flow heat transfer and component transfer process in the pulverized coal combustion process. The model serves as a reference for the practical application of TRI in pulverized coal boiler combustion research.

## RESULTS AND DISCUSSION

**Simulation Method and Model Verification. Turbulence Model.** In this paper, mass, momentum, energy, and component transport equations are considered in the calculation process. The realizable k−ε model is used to describe the turbulent flow in the 300 MW tangentially fired pulverized coal furnace.

**Combustion Model.** For combustion of pulverized coal in the furnace, we considered processes such as inert heating, moisture evaporation, devolatilization, and coke combustion. In FLUENT, we used the default Custom law to achieve these processes. We used the β-PDF model to calculate the effects of combustion component fluctuation; coke combustion uses a power/diffusion model; the volatile precipitation model adopts the chemical percolation devolatilization (CPD) model; for the volatile composition required in the cracking process, please refer to the literature; the soot generation is presented in the following sections.

**Soot Generation Model.** Most of the current research studies on the formation and oxidation of soot are built on simplified soot models. It is commonly used because of its advantages such as easy implementation and low calculation cost. However, this method of describing the soot generation and oxidation processes is too simplified, ignoring the effects of surface growth, collision condensation, and surface deposition of soot particles on soot formation. In order to accurately predict the formation of soot, the PBM is used to describe the detailed process of soot formation. The evolution of soot particles can be expressed by the population balance equation

\[
\frac{\partial n(L; x, t)}{\partial t} + \frac{\partial}{\partial x_i}(u_i n(L; x, t)) = \frac{\partial}{\partial x_i} \left[ (\Gamma + \Gamma^{\delta}) \frac{\partial n(L; x, t)}{\partial x_i} \right] = S(L; x, t)
\]

where \( L \) represents the characteristic length of the particle and in this calculation, refers to the particle size; \( \Gamma \) is the molecular diffusivity; \( \Gamma^{\delta} \) is the turbulent diffusivity. For turbulent flow \( \Gamma^{\delta} \gg \Gamma \), it is generally believed that \( \Gamma + \Gamma^{\delta} \approx \Gamma \); \( x \) and \( t \) represent space position and time, respectively. \( S(L; x, t) \) represents the source term, including the nucleation, surface growth, oxidation, and agglomeration processes of the soot.

The number of particles \( n(L; x, t) \) can be expressed using the Dirac function, that is

\[
n(L; x, t) = \sum_{\alpha=1}^{N} a_{\alpha}(x, t) \delta(L - L_{\alpha})
\]

In order to reduce the amount of calculation, instead of directly solving the number of particles but solving the distribution moment of the number of particles, the distribution moment of the number of particles can be approximated by a summation
in the fuel-rich area. Because of the lack of oxygen in this area, a large amount of tar will be quickly converted to soot. In this process, the evolution of soot includes nucleation, agglomeration, surface growth, and oxidation processes. From the primary product of coal combustion, the small-molecule PAH begins to condense into a nucleus as initial soot, after which the main gas-phase PAH attached to the soot grows and then undergoes collision agglomeration and oxidation in OH and O. Saggese research shows that nucleation is mainly a small-molecule benzene ring. Depending on CPD calculation, we assume that the precursor $X_{\text{prec}}$ generated by soot is the benzene ring $C_{6}H_{6}$.

The mathematical model is as follows

$$ S_{k} \approx S_{k}^{(N)} = r_{\text{g}} + r_{\text{ad}} + r_{\text{fg}} - r_{\text{inc}} $$

**Nucleation Models.** The nucleation process is mainly the nucleation of precursors of a certain rate of the calculation domain. The nucleation rate $J$ must be considered.

$$ r_{\text{inc}} = \frac{k_{n}^{N}}{k} J(x, t) $$

$$ J \approx N_{\text{av}}^{2} T^{1/2} \times 10^{6} \exp \left( -\frac{46,100}{T} \right) X_{\text{prec}} $$

**Surface Growth of Soot Particles.** After the soot particles are nucleated, the soot particles will absorb the precursors and continue to grow, assuming that $G(L)$ is the continuous rate of particle change and molecular surface growth rate

$$ r_{\text{g}} = k \int_{0}^{+\infty} L^{k-1} G(L) n(L) \, dL $$

$$ G_{\text{ag}} = \frac{6}{\rho D_{L}} \left( \frac{L_{C}}{L_{C0}} \right)^{3-D_{L}/3} M_{G} \times 6 \exp \left[ -\frac{6083}{T} \right] X_{\text{prec}} \right) $$

**Soot Particle Agglomerates.** Particle agglomeration is mainly caused by the collision of two particles of different sizes. The formula is as follows

$$ r_{\text{ag}} = \frac{1}{2} \int_{0}^{+\infty} (L_{1} + L_{2})^{3-k} \beta(\mu, \mu) \times \hat{n}(L_{1}) \hat{n}(L_{2}) \, dL_{1} \, dL_{2} $$

$$ - \int_{0}^{+\infty} \int_{0}^{+\infty} L_{1}^{3} \beta(\mu, \mu) \times \hat{n}(L_{1}) \hat{n}(L_{2}) \, dL_{1} \, dL_{2} $$

**Soot Particle Oxidation.** We use the oxidation model proposed by Brown and Fletcher, and the specific calculation formula is as follows

$$ r_{\text{OC}} = S_{A} V_{C} C_{OC} \frac{P_{O_{2}}}{T^{1/2}} A_{\text{OC}} e^{-E_{\text{OC}}/RT} $$

$$ S_{A} V_{C} = \left( 6^{3/3} \pi^{1/3} \left( \rho_{C} N_{C} \right)^{3/3} Y_{C}^{2/3} \rho^{2/3} / \right) \rho_{C}^{2/3} $$

**Radiative Heat Transfer.** Radiative heat transfer plays a large role in the combustion of the boiler furnace and can be described by the radiation transfer equation, which considers the radiation and scattering of pulverized coal. The radiative transfer equation (RTE) can be written as follows

$$ \frac{dI(\vec{r}, \vec{s})}{d\Omega} = k_{g} I_{\text{g}} + E_{p} - (k_{g} + k_{p} + \delta_{p}) I_{s}(\vec{r}, \vec{s}) $$

$$ + \frac{\delta_{p}}{4\pi} \int_{0}^{2\pi} I_{s}(\vec{r}, \vec{s}') \phi(\vec{s}, \vec{s}') \, d\Omega $$

**Table 1. Transport Equation Source Terms**

| term | $A$ | $E$ (kJ/g-mol) | source |
|------|-----|---------------|--------|
| $r_{\text{inc}}$ | 1.09 $\times 10^{6}$ (K$^{1/2}$/s) | 164.5 | Brown and Fletcher |
where $I_b$ is the black body intensity and $\phi(\overrightarrow{s}, s')$ is the scattering phase function.

$E_p$ is the equivalent particle emission and $k_p$ and $\sigma_p$ are the equivalent particle absorption and scattering coefficients over a given volume $V$, respectively, as follows

$$E_p = \frac{1}{V} \sum_i Q_{abs,i} A_{p,i} \rho_{p,i}(T_{p,i})$$  \hspace{1cm} (17)

$$k_p = \frac{1}{V} \sum_i Q_{abs,i} A_{p,i}$$  \hspace{1cm} (18)

$$\sigma_p = \frac{1}{V} \sum_i Q_{sca,i} A_{p,i}$$  \hspace{1cm} (19)

In this paper, the DOM with gray body assumption for gas and particle properties is selected for the radiative heat transfer. Considering the balance between the cost of the simulation and accuracy of predicting the thermal radiation, the DOM with $3 \times 3$ angular discretization is used.

The WSGG model, which can achieve a high level of accuracy with smaller computational requirements, where the gas is as follows

$$k_{CO_2+H_2O} = \sum_{i=0}^{3} a_{g_i} i_g(T)(1 - \exp(\kappa_{g_i} \sqrt{i_g C_{CO_2} + P_{H_2O}} L))$$  \hspace{1cm} (20)

$$a_{g_i} i_g(T) = \sum_{j=0}^{3} h_{g_j} i_g j^p, \ \ \ i_g = 0,1,2,3$$  \hspace{1cm} (21)

Fitting factor $h_{g_j}$ is derived from the literature ref 47.

According to the MIE theory, Yang calculations found that the coefficient of scattering of pulverized coal particles is essentially constant during combustion. We consider the radiation effect of pulverized coal particles and set the emissivity of pulverized coal particles to 0.85 in the discrete-phase method (DPM) calculation. 48

Soot agglomeration in the flame is very small, $\pi dp/\lambda \ll 1$, so we neglected scattering. The soot absorption coefficient is

$$k_{soot} = 1.644 \times 10^{3} f_{soot} T$$  \hspace{1cm} (22)

We add this refined absorption coefficient to the FLUENT using the user-defined function (UDF).

**TRI Model.** In this paper, eq 23 is time-averaged with the scattering term removed. The reason is that when using the DPM model to simulate particle combustion, the discrete random walk (DRW) model in the DPM can be used to consider the fluctuation of the particles. The time-averaged radiation equation can be obtained as follows

$$\frac{df}{dt} = -k + k_b$$  \hspace{1cm} (23)

$$k = k_{CO_2+H_2O} + k_p + k_{soot}$$  \hspace{1cm} (24)

During the combustion of pulverized coal, the thin optical pulsation approximation assumption suitable for most engineering applications is adopted. The first term of the right side of eq 25 can be ignored without considering pulsation correlation, so we get the time-averaged furnace radiation equation.

$$\frac{df}{dt} = -k + k_b$$  \hspace{1cm} (25)

The second term on the right side of formula 26 is proportional to $kT^4$ so that the autocorrelation of the absorption coefficient is ignored, and the instantaneous variable is decomposed into $T = T + T' \kappa = \bar{K} + \kappa'$.

$$kT^4 = (\bar{K} + \kappa')(T + T')^3$$  \hspace{1cm} (26)

Figure 2. Schematic of implementation of the coal combustion model in FLUENT.
By ignoring the effect of other higher-order terms, eq 27 is simplified.

\[
\overline{k T^4} = \kappa \cdot T^4 \left( 1 + C_{\text{TRI}} 4 \frac{T^2}{T^2} + C_{\text{TRI}} 4 \frac{T^2}{T} \frac{\partial k}{\partial T} \right)
\]

(27)

Here, TRI is added to ANSYS FLUENT’s energy equation through a UDF. FLUENT provides time-integrated variables that include the square of the solution variable. The value of any variable (such as \( T^2 \)) can be obtained. The expression in parentheses in eq 26 takes into consideration turbulent fluctuations. The second term in the brackets \( C_{\text{TRI}} 4 \frac{T^2}{T} \) is called the temperature autocorrelation term, and the third term \( C_{\text{TRI}} 4 \frac{T^2}{T} \frac{\partial k}{\partial T} \) is called the absorption temperature-dependent term.

The approximation of \( \overline{k T^4} \) is obtained from eq 26. For the RANS solution, one can use a presumed PDF for temperature pulsation to obtain the pulsation value of \( \frac{\partial k}{\partial T} \). Burn et al. investigated the effect of component scales in PDF on temperature self-correlation, yielding values between 0 and 2.5 for \( C_{\text{TRI}} \). Using PF-PDF, \( C_{\text{TRI}} \) values suitable for furnace pulverized coal combustion can be obtained for component distribution coefficients at different locations. \( C_{\text{TRI}} 4 \frac{T^2}{T} \frac{\partial k}{\partial T} \) is the absorption temperature-dependence term and has a small influence because of the inclusion of the derivative \( \frac{\partial k}{\partial T} \), which in this paper is set to \( C_{\text{TRI}} \) of 1.

The implementation method and calculation processes of the pulverized coal combustion and soot formation model on the FLUENT platform are shown in Figure 2 below.

This diagram illustrates our entire calculation process. In the mathematical model, we use the realizalbe \( k-e \) model, and the scalable wall function is used to predict the velocity and temperature distributions at the nearest grid from the wall surface. For the particle combustion model, the DPM is used to compute the particle trajectories. To consider turbulent dissipation of the particles, the discrete random walk (DRW) model is added. In the DPM model, the time scale constant is equal to 0.3, and the number of attempts is same as 5.4. The coal particle size distribution uses the Rosin-Rammler distribution, and the average particle size is 35 µm.

The CPD model is used for devolatilization. Moreover, for coke combustion, we use the power and diffusion models. In the soot production model, the PBM is applied, in which nucleation, growth, agglomeration, and oxidation models are added to FLUENT with the UDF. In terms of radiant heat transfer, the soot coefficient is added to the UDF. Similarly, in the DOM model, the UDF is used to hook TRI and the radiation model.

**Soot Generation Model Validation and Their Key Parameter Analysis.** In order to verify and analyze the soot mathematical model in this paper, we used the newly established soot generation model to simulate the characteristics of the pulverized coal combustion field formed by the 4 kW jet burner of Central Research Institute of Electric Power Industry (CRIEPI). \(^{51}\) for the details of the set and physical model, please see refs 52 and. \(^{53}\) Figure 3 is a comparison between the numerical simulation diagram and the experimental photographs. The beginning combustion position of the simulated flame is also at the height of the burner (HAB) = 30 mm. As the flame temperature gradually extends, the peak temperature reached about 2100 K at HAB = 80–140 mm (the maximum temperature of the simulated flame is 2091 K). At HAB = 180 mm, the flame temperature is reduced to about 1800 K. It can be seen from the comparison that the simulation results are basically consistent with the experimental results.

The distributions of \( c(s) \) (fixed carbon), soot oxidation rate, soot nucleation rate, and soot volume fraction are displayed in Figure 4. The pyrolysis of the fixed carbon starts at a lower position, and after that, fixed carbon increases gradually from the flame, in Figure 4. With more and more fixed carbon particles in the height direction, the oxidation rate and nucleation rate of soot gradually increase, so the volume fraction of soot is also the largest, which is consistent with the test results.

Figure 5 is an experimental \(^{54}\) and simulated comparison of the cumulative frequency of the primary soot particle diameter based on particle volume. In Figure 5, as the height increases, the diameter distribution of primary soot particles shifts to the larger side. This trend indicates that as the particles move below the burner, the primary soot particles grow. The growth of primary soot particles is achieved by the addition of gas-phase molecules and the condensation of soot particles. The study found that with the increase in height, the distribution of primary soot particle diameter becomes wider and wider, which is also consistent with the experiment. \(^{52}\)

Figure 6 is a comparison of the radial distributions for the simulated soot volume fraction and experimental results \(^{50}\) of the L II signal. It can be observed in the figure that the soot volume distribution is similar to the peak value of the signal measured in the experiment, and this is consistent with the experimental result of the optical signal measurement. Considering the effect of TRI, soot production is higher.

In this paper, \( \text{C}_6\text{H}_6 \) was used as a precursor for soot nucleation. Compared with Takahashi’s simulated results which used the small-molecule gas as precursors in 48, the peak value of the soot volume fraction we calculated is closer to the experimental peak point because the small-molecule gas generally volatilizes first, and then, the precursor appears. Consider that the OH oxidation function was ignored in our calculation process, \(^{50}\) so compared with the experiment, there still exists an error compared with the experimental results, but overall, it shows that the results of this model are reasonable and can be used in the subsequent pulverized coal combustion simulation of the furnace.

After the soot particles are nucleated and grown, they will collide, coagulate, and agglomerate further, and the particle
clusters formed through these processes are known as agglomeration. The agglomeration body has a self-similar structure, that is, a typical fractal structure. Therefore, using fractal dimensions ($D_f$) to study soot particles can more accurately predict soot generation. As can be seen from Figure 7, according to the SEM results of the Central Research Institute of Electric Power Industry (CRIEPI), the fractal dimension of soot agglomeration was calculated based on the difference box dimension method, and the $D_f$ range was 1.481−1.6091. Therefore, in this paper, the $D_f$ value in the calculation of pulverized coal combustion was chosen to 1.56.

Simulation and Analysis in the Pulverized Coal Combustion in the Boiler Furnace Using These Mathematical Models. Physical Model Introduction. This paper takes a 300 MW boiler furnace as the research object. The coal type is Mengdong Baiyinhua lignite, and coal quality analysis results are shown in Table 2. The dimensions of the furnace are 60 m height, 14.048 m width, and 14.019 m depth. The burner nozzles are arranged alternately, and they are arranged from the bottom to the top as follows: 2-1-2-1-2-2-1-2-1-2-the separated over fire air (SOFA) (2 is the secondary air nozzle and 1 is the primary air nozzle), and the boiler structure is shown in Figure 8.

Meshing Introduction. A three-dimensional model is established using ICEM software, and the meshing of the boiler furnace model is shown in Figure 9. Encrypt the combustion area accordingly. The total number of grids is 1.98 million, and the quality is good.

Because the structural grid division of the boiler is comparatively complex, this article only carried out four grid divisions, and the number of cells in the grids was 1.52 million, 1.77 million, 1.98 million, and 2.21 million. Because the effect of TRI affects temperature, temperature is observed under the same working conditions, and the detected surfaces are 2, 8, 15, 20, and 40 m. As can be seen from Figure 10, the temperature distribution results of 1.98 million grids and 2.21 million grids are relatively close. When the grid density is low (1,529,576 and

Figure 4. Distributions of $c(s)$, soot oxidation rate, soot nucleation rate, and soot volume fraction [(a) $c(s)$, (b) soot oxidation rate, (c) soot nucleation rate, and (d) soot volume fraction].

Figure 5. Experimental and simulation comparison of cumulative frequency of the primary soot particle diameter ($h = 35$ mm and $h = 95$ mm).

Figure 6. Comparison of the radial distributions for the simulated soot volume fraction and experimental results of the L II signal (the black dotted line indicates the simulated results from Hayashi, the red dotted line indicates the simulated results from not considering TRI, and the blue triangular line indicates the simulated results from considering TRI).

Figure 7. Fractal dimension calculation results based on the SEM results of CRIEPI (fractal dimension $D_f$ is the slope).
From the perspective of calculation accuracy and calculation efficiency, this paper decides to choose the third grid division scheme, that is, the number of cells in the grids is 1.98 million.

**Relevant Working Condition Settings for Simulation.** By simulating the combustion process of the furnace under three different boiler loads (140, 210, and 300 MW), the TRI effects on furnace combustion, soot, and NOx emissions were studied. The following working conditions 1, 2, and 3 are meant to the simulation boiler loads of 140, 210, and 300 MW, respectively, which are the conditions without considering the action of TRI, and the working conditions 4, 5, and 6 are meant to the boiler loads of 140, 210, and 300 MW, respectively, which are the conditions with considering the action of TRI. The specific parameters of each load are shown in Table 3.

**Comparison and Verification of Simulation and Power Plant Data.** To verify the results of numerical simulation, we collected three sets of data of the furnace’s outlet from the measurement system of the 300 MW boiler. Table 4 shows the comparison between the simulated values and the measured data. It can be seen that the simulated values (considering TRI) of the furnace outlet under the different loads are closer to the measured data. The temperature error between the simulation and the measure is within 0.56%. Moreover, without considering TRI, the error is within 5.14%. Therefore, the mathematical models for this simulation are reasonable and reliable and can be applied to the simulation calculation of relevant pulverized coal combustion.

**Table 5** shows the comparison of temperatures at the furnace outlet calculated by taking into account different TRI factors. According to the previous section, under the thin optical assumption, the first part of TRI eq 19 temperature self-correlation can be represented entirely by the properties of the pdf function $P(f)$. The study used different distributions, and the analysis yielded coefficients for $C_{TRI1}$ ranging from 0 to 2.5. In this paper, three values of 1.5, 2.0, and 2.5 were taken for comparison using the $\beta$-pdf function, and the calculations showed that 2.0 was more consistent with the test data, and 2.0 was used for subsequent analysis.

**Simulation Results and Analysis.** *Effect of TRI on Temperature Field.** Figure 11 shows the average temperature distribution of the longitudinal section of the furnace under different conditions, whether considering TRI or not. Comparing the working conditions 1 (Figure 11a) and 2 (Figure 11d), the peak value of the average flame temperature of the furnace section (Figure 11a) is 1550 K when TRI is not considered. When TRI is considered (Figure 11d), the peak value of the average flame temperature of the furnace section is 1477 K. Comparing the working conditions 2 (Figure 11b) and 5 (Figure 11e), when TRI is not considered (Figure 11b), the peak value of the average flame temperature is 1559 K. Comparing the working conditions 3 (Figure 11c) and 6 (Figure 11f), the peak value of the average flame temperature of the cross section of the furnace is 1609 K. This indicates that the temperature is relatively large. From the perspective of calculation accuracy and calculation efficiency, this paper decides to choose the third grid division scheme, that is, the number of cells in the grids is 1.98 million.

**Table 2. Results of the Coal Quality Analysis**

| proximate analysis (%) | ultimate analysis (%) | lower heating value $Q_{net,ar}$ |
|-----------------------|-----------------------|-------------------------------|
| $W_{ar}$ | $A_{ar}$ | $V_{ar}$ | $F_{C_{ar}}$ | $C_{ar}$ | $H_{ar}$ | $O_{ar}$ | $N_{ar}$ | $S_{ar}$ | 14.91 |
| 14.2 | 19.038 | 32.9 | 33.862 | 39.434 | 3.53 | 8.846 | 0.672 | 0.402 | 14.91 |

**Figure 8.** Arrangement of nozzles of the 300 MW tangentially fired boiler furnace structure.

**Figure 9.** Meshing of the boiler furnace model.

**Figure 10.** Temperature distribution at different heights in the same boiler load (140 MW).
condition 6), respectively. It can be seen that as the boiler load increases, the overall furnace temperature also increases. In contrast with the simulated conditions with and without TRI, the average flame temperature peaks at the furnace section decrease by 73, 47, and 58 °C, respectively. It can be seen that the overall furnace temperature when TRI is considered will be reduced accordingly.

Figure 12 is the curve of the average temperature of the cross section of the furnace along the height of the furnace under different working conditions. It can be seen from the figure that the average temperature along with the furnace height is relatively reduced, while TRI is considered (working condition 4, 5, and 6), and the trends are generally consistent. The temperature in the primary combustion area is distributed in a

Table 3. Parameters of Working Conditions

| boiler load (MW) | primary air speed (m/s) | primary air temperature (K) | secondary air speed (m/s) | secondary air temperature (K) | SOFA speed (m/s) | SOFA temperature (K) |
|-----------------|-------------------------|----------------------------|--------------------------|-------------------------------|-----------------|---------------------|
| 140             | 17.52                   | 338                        | 48                       | 662                           | 42              | 662                 |
| 210             | 19.36                   | 338                        | 48                       | 662                           | 44              | 662                 |
| 300             | 25.07                   | 338                        | 48                       | 662                           | 47              | 662                 |

Table 4. Comparison between Numerical Simulation Results and Power Plant Measurement System’s Data

| boiler load (MW) | parameter | data from the measurement system | simulation value (considering TRI) | simulation value (without considering TRI) |
|-----------------|-----------|----------------------------------|------------------------------------|------------------------------------------|
| 140             | temperature/K | 1220                             | 1218/0.16%                         | 1256/2.9%                                |
|                 | O₂ concentration/% | 4.03                             | 4.01                               | 4.25                                     |
|                 | NOₓ concentration/mg·Nm⁻³ | 466.88                           | 464.73                             | 486.34                                   |
| 210             | temperature/K | 1244                             | 1237/0.56%                         | 1289/3.62%                               |
|                 | O₂ concentration % | 4.44                             | 4.33                               | 4.38                                     |
|                 | NOₓ concentration/mg·Nm⁻³ | 570.2                             | 566                                | 577.78                                   |
| 300             | temperature/K | 1265                             | 1270/0.4%                          | 1330/5.14%                               |
|                 | O₂ concentration % | 4.53                             | 4.58                               | 4.61                                     |
|                 | NOₓ concentration/mg·Nm⁻³ | 621                              | 633                                | 650                                      |

Table 5. Comparison Table between Numerical Simulation Results in the Value of C_TR1 and Power Plant Test Data

| boiler load (MW) | parameter | power plant data | numerical simulation (C_TR1 = 2.5 | numerical simulation (C_TR1 = 2.0 | numerical simulation (C_TR1 = 1.5 |
|-----------------|-----------|------------------|-----------------------------------|-----------------------------------|-----------------------------------|
| 140MW           | temperature/K | 1220             | 1203                              | 1218                              | 1249                              |

Figure 11. Average temperature distribution of the longitudinal section of the furnace under different conditions whether considering TRI or not. (a) Working condition 1. (b) Working condition 2. (c) Working condition 3. (d) Working condition 4. (e) Working condition 5. (f) Working condition 6.
zigzag manner because of the interval distribution of the primary and secondary air nozzles. The maximum temperature difference along with the furnace height are 80 °C (compare working condition 1 and working condition 4), 95 °C (compare working condition 2 and working condition 5), and 97 °C (compare working condition 3 and working condition 6), and the average differences are 57 °C (compare working condition 1 and working condition 4), 51 °C (compare working condition 2 and working condition 5), and 54 °C (compare working condition 3 and working condition 6). From Figures 11 and 12, it is shown that TRI is significant to the radiant heat transfer of the furnace and the efficient use of energy.

Effect of TRI on O2, CO, and NOx. The O2 and CO mole fractions of the furnace had a considerable effect on the reducibility in the furnace, which has a positive influence on NOx and soot generation. Figure 13 is the distribution of the average oxygen concentration of the cross section of the furnace along with the furnace height. It can be seen from the Figure 13 that the trend of O2 concentration changes with the height of the furnace under each working condition and is basically the same; they all increase first, then zigzag, and finally stabilize. However, as the load increases, the amount of pulverized coal will also increase. To fully burn the pulverized coal, the increase in the amount of air supply will cause the O2 concentration of the section to increase slightly. Because of the reduction of radiative heat transfer of the furnace after considering the effect of TRI, combustion is relatively inadequate under the same conditions, which will cause a slight decrease in O2 consumption. Therefore, after considering TRI, the O2 concentration slightly increases, but the difference is small.

Figure 14 shows the average CO mole fraction distribution along the furnace height whether TRI is considered or not. It can be seen that the overall level of the mole fraction of CO increases from the increase in the furnace height and gradually declines after 20 m and decreases to 0.1% at the furnace outlet. It shows that in the flame center region (15−20 m), the proportion of incomplete combustion of pulverized coal is large. The temperature in this region is also the highest, so NOx and soot are easy to generate in this region (15−20 m). Simultaneously, as the boiler load increases, the overall temperature of the furnace increases, and pulverized coal combustion is dominated by secondary reaction and rapidly produces CO, so the molar fraction of CO is relatively increased. When TRI is considered, the overall temperature decreases and its CO increases slightly.

There are three main types of NOx formation of the combustion of pulverized coal: thermal NOx, fast NOx, and fuel NOx. Because the fast NOx has a small proportion compared with the other two types, the main consideration used for this simulation is the remaining two types of NOx. Figure 15 is the distribution of the average NOx concentration distribution of the cross section of the furnace along the furnace, considering TRI or not. As can be seen from Figure 15, NOx emissions increase with increasing load. NOx concentration is reduced when TRI is taken into account. This is because the overall temperature calculation of the furnace is smaller when TRI is taken into account, resulting in a reduction in NOx production.

Effect of TRI on Soot Concentration of the Furnace. The lower the load, the less complete the combustion and the higher the impact on soot generation. Therefore, this paper analyzes the soot produced when the boiler load is 140 MW (working condition 1 and working condition 4). Figure 16 shows the average soot density distribution of the cross section of the furnace in 15 m height. As can be seen from Figure 14, soot is mainly found in the mid and downstream regions of the flame. The effect of TRI does not change the overall distribution trend, but the average temperature is 67 °C higher without considering TRI than with TRI; however, the average concentration of soot
increases by 1.524 g/m³ when the TRI effect was considered, which indicates that the relationship between temperature and soot generation is negatively related. Therefore, it can be seen that considering TRI will increase the amount of soot generation.

The circle positions are drawn in Figure 16a,b and correspond to the high-temperature zone and the low oxygen concentration zone. This zone is heavily cracked to produce tar from coal dust, but a high number of soot is produced because of insufficient oxygen, as shown in the circle in Figure 16c. After considering the TRI effect, the temperature shown in Figure 16d was reduced compared to Figure 16a. The oxidation reaction rate slows down, and the soot generation concentration increases compared to Figure 16c.

Effect of TRI on the Process of Intermediate Products of Soot. Figure 17 is a graph showing the change in the percentage of coal char mass, soot nucleation, soot oxidation rate, and soot volume percentage along with the height under the action of TRI. It can be seen from the figures that under the action of TRI, the overall trends of the intermediate process value such as the coal char rate, soot nucleation rate, and oxidation rate are first increased and then decreased, and soot volume also has this trend. At the furnace height of 19−22 m, the mass percentage of coal coke, soot nucleation, and soot oxidation rate suddenly dropped. It can also be seen from the soot volume fraction that it
plummets from 19 to 22 m. Figure 18 is a graph showing changes in the volume fraction of soot along with the height under the action of TRI or not. It can be seen from Figure 18 that the soot volume fraction increases first and then decreases with the furnace height. When considering the effect of TRI, the soot volume is a relatively more amount. This is because when the overall temperature of the furnace is lower under the consideration of TRI, the temperature is negatively correlated with the soot generation (verified above), so the amount of soot generated is greater when TRI is considered. Temperature has a great influence on the combustion of pulverized coal, such as the volatilization rate of coal particles, the reaction rate of volatiles, the percentage of coal char mass, soot nucleation, soot oxidation rate, and pollutants (such as NO and soot). Therefore, it is necessary to consider the influence of TRI.

Turbulent pulsation is caused by the local fluid movement (including composition, temperature, etc.) affecting the heat radiation transfer, which in turn affects global combustion. Figure 19 shows the distribution of volumetric emitted radiation along the height whether considering the effect of TRI or not. Considering the TRI effect (as shown by the red dotted line in Figure 19), the carbon smoke influence extends over a larger area, resulting in a larger magnitude of the volumetric emission radiation curve. However, in the bottom and top regions of the furnace, TRI has less influence on the volume emission radiation.

**CONCLUSIONS**

This paper takes the 300 MW pulverized coal combustion furnace as the research object and establishes a mathematical model of turbulent combustion of pulverized coal suitable for engineering research. The model is used to simulate the
combustion process in the furnace and the generation of smoke and NOx under different boiler loads. The result is as follows:

(1) A simplified soot evolution model for pulverized coal combustion is established. In this model, C6H6 is used as the precursor of soot generation, and the evolution process of soot nucleation, growth, agglomeration, and oxidation is also included. The TRI model is established during pulverized coal combustion.

(2) Studies have shown that soot production is affected by external flow and radiation. Collision aggregation requires the consideration of particle flocculation. For engineering applications, fractal dimensions can be used, with an estimated value of 1.55. The β-PDF function was used to solve TRI, and the CTRI, coefficient of 2.0 was more realistic for high-temperature furnace combustion.

(3) TRI has a significant impact on temperature changes and soot and NOx formation. The soot volume is negatively related to temperature. After considering the effect of TRI, the maximum changes in the average cross-sectional temperature were 80, 95, and 97 °C; the average temperature differences from the average TRI cross section without consideration were 57, 51, and 54 °C. The NOx content is relatively reduced. Considering TRI at 140 MW, its soot concentration increased.

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■ SYMBOL DESCRIPTION

Γ molecular diffusivity
Γt turbulent diffusivity
ωa weight function of the feature length
N orthogonally approximated nodes
k order of moments
ε nucleation diameter, m
NA Avogadro constant
ρ gas density, m3/kg
Xprec precursor molar volume, mol/m3
Vi group i particle volume, m3
kB Boltzmann constant, J/K
ρs relative particle density, kg/m3
ν kinematic viscosity coefficient of fluid, m2/s
T absolute temperature, K
Ψkj collision efficiency
βc clustering rate, m3/s
βs turbulent cluster nuclei, m3/s
V collision nuclear volume, m3
u collect nuclear volume, m3
L particle diameter, m
Dt fractal dimension
P0 partial pressure of oxygen
Nc soot particles per unit mass
ωC carbon mass fraction
E emission, W/m3
k Planck absorption coefficient
n the number of particles
x space position, m
t time, s
S the source term
δ delta function
ω weight function of the feature length
m the distribution moment of the number of particles
Lc particle collision radius, m
R universal gas constant
Y mass fraction
SA total surface area, m2
Aproj projected surface area of particle i, m2
I radiation intensity, W/(sr m3)
E activation energy
κ absorption coefficient, 1/m
κp particle absorption coefficient, 1/m
σp particle scattering coefficient, 1/m
Qnet lower heating value
W moisture

■ SUBSCRIPT

pre precursor
nc condensation
ag conglomerate
gl grow
oc oxidation
i 1 granules
tur turbulent motion
bro Brown motion
m turbulent motion
f gas
ffc c

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