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Effects of Turbulent Mixing and Controlling Mechanisms in an Entrained Flow Coal Gasifier

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There is a large range of time and length scales of turbulent fluctuations in an entrained flow coal gasifier. To figure out the turbulent effects on coal gasification processes and the controlling mechanisms of different regions in an entrained flow coal gasifier, the characteristic time and length scales for all major processes are estimated. On the basis of the comparison between the length/time scales of turbulent mixing in all ranges and the characteristic time of homo- and heterogeneous reactions, turbulent effects on reactions and coal gasification processes in different regions in an entrained coal gasifier are studied. In the flame region, there is a strong coupling effect between macro-scale turbulent fluctuation and heterogeneous reactions. The combustion of the volatile is strongly affected by the fluctuation of micro-scale Kolmogorov scales because the diffusion boundary layer of the particles is destroyed by this kind of fluctuation. In the nonflame region, the heterogeneous char gasification reactions are not affected by turbulent fluctuations; however, the coupling effect between turbulent mixing and gas-phase reactions should not be omitted.

1. Introduction

Entrained flow coal gasifiers have been widely used in coal gasification technologies because of their high capacity and steady good performance. In such kinds of gasifier, coal or coal slurry particles are usually injected into the furnace with pure oxygen at a high speed. The elevated pressure and high temperature in the gasifier guarantees a high carbon conversion in a short residence time. The gasification process in an entrained flow coal gasifier is very complex. A series of physical and chemical processes happen on the coal slurry particles, such as evaporation of water, pyrolysis of coal, and heterogeneous coal char reactions. At the same time, there are strong coupling effects among turbulent fluctuaction, chemical reactions, and heat transfer to particles. Especially, temperature and local velocities have a strong influence on these coupling effects, which makes the controlling mechanism and turbulent fluctuaction effects change at different regions of an entrained flow gasifier. To deeply understand the gasification process, it is important to figure out the controlling mechanisms and turbulent effects in the gasifier.

On the basis of experimental and modeling studies, a lot of analysis has put focus on this topic. In the modeling work of Wen and Chuang,[1] the entrained flow coal gasifier is divided into three zones: the pyrolysis and volatile combustion zone, the gasification and combustion zone, and the gasification zone. In each zone, different controlling mechanisms are considered, so that the model can depict the real gasification process better. Soelberg et al. and Smoot and Brown studied the mixing and reaction processes and controlling mechanisms within a laboratory-scale entrained coal gasifier at atmospheric pressure,[2,3] through analysis of experimental data and by a comparison to predictions of a comprehensive model. They proved the existence of three regions of mixing and reaction in the gasifier. The coal heat up and devolatilization occur rapidly near the coal inlet region. Oxygen and volatile yielding out are consumed in this region in a short time, producing a high gas temperature and high CO_2 concentration. Heterogeneous coal char reactions are controlled in this region through oxidizer diffusion to the char surface. Outside this region, however, as the temperature declines, the heterogeneous char−oxidizer reaction near the particle external surface becomes more important. Through a 3D numerical simulation for an entrained flow coal gasifier,[4] Liu et al. investigated the effect of mixture fraction fluctuations on the overall gasification characteristics as a result of turbulent flow. It was found that turbulent fluctuation has a strong effect on the devolatilization process and char−oxygen reactions, while the char reactions with H_2O and CO_2 are not affected by the turbulent fluctuation apparently.

The main objective of this paper is to give a systematic analysis on the turbulent fluctuation effects and the controlling mechanisms in an entrained flow coal gasifier based on comprehensive numerical simulation and fundamental turbulent theories. The length and time scale distributions of large and small eddies are compared to the characteristic time of homo- and heterogeneous reactions. Turbulent effects on

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(1) Wen, C. Y.; Chuang, T. Z. Entrainment coal gasification modeling. *Ind. Eng. Chem. Process Des. Dev.* **1979**, *18* (4), 684–695.

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Table 1. Length and Time Scales of Different Eddies and Reynolds Number Averaging Turbulence Information[5,6]

	integrate scale	Taylor scale	Kolmogorov scale
length scale	$L_L = k^{3/2}/\varepsilon$	$L_\lambda = (10k\nu/\varepsilon)^{1/2}$	$L_\eta = (\nu^3/\varepsilon)^{1/4}$
time scale	$\tau_L = k/\varepsilon$	$\tau_\lambda = (15\nu/\varepsilon)^{1/2}$	$\tau_L = (\nu/\varepsilon)^{1/2}$
Re	$Re_L = k^2/\varepsilon\nu$	$Re_\lambda = k/(3\varepsilon\nu/20)^{1/2}$	1

reactions and coal gasification processes in different regions in an entrained coal gasifier are studied.

2. Theoretical Analysis of Time and Length Scales

2.1. Turbulent Theory of Length and Time Scales. Turbulence is characterized by fluctuations of all local properties in a large range of time/length scales and occurs for sufficiently large Reynolds numbers. For homogeneous isotropic turbulence, the energy of the large scales flows to the smaller scales through the Kolmogorov cascade. The energy flux from one scale to another is constant along scales and is given by the dissipation ε of the kinetic energy k. Along the cascade, the turbulent Reynolds number goes down from Re_t to values to unity. The turbulent Reynolds number, Re_t, is given by

$$Re_t = u'l_t/\nu \tag{1}$$

where u' is the velocity fluctuation, l_t is the characteristic length of the large eddies, which are in the same magnitude as the characteristic length of geometry, and ν is the kinematic viscosity of the turbulent flow.

In turbulent flows, there are usually three scales that are important to identify the mixing and fluctuation of turbulence. The integral time or length scales characterize the larger eddies in the flow, which are generally regarded to depend upon the geometry and initial conditions. The integral scales of turbulence fluctuation (or eddies) have a strong effect on the flow pattern in the macro-scale. Kolmogorov scale, η_k, determines the smallest scale found in the turbulent flow. In this scale, inertia and viscous forces balance and molecular diffusion occurs as well as chemical reactions. As a result, the chemical source terms for some reactions will be strongly coupled to the turbulent mixing process. It is the main task in this paper to figure out which reactions are strongly coupled to the turbulent mixing process in each typical region in a gasifier. Other widely used length scales are the Taylor micro-scales, which are often used to characterize the magnitude or intensity of the turbulence.

All three of these typical scales can be identified by the statistics information of the turbulent flow, for e.g., k and ε. These relationships are shown in Table 1, where the characteristic length, time, and Reynolds number for each scale are represented by k, ε, and the kinematic viscosity ν.

On the basis of equations given by Table 1, the main features of the turbulent fluctuation in all scales in an entrained flow coal gasifier can be found as long as the statistics are acquired through a classical 3D numerical simulation with Reynolds-averaged Navier−Stokes (RANS) method. The simulation work will be depicted in the next section.

2.2. Three-Dimensional Numerical Simulation of an Entrained Coal Gasifier. A comprehensive three-dimensional numerical model was proposed for the simulation of entrained coal gasifiers. In this model, a presumed probability-distribution function (PDF) method was used to describe the turbulent reaction and turbulent mixing process of the gas phase in the gasifier. A realizable $k−\varepsilon$ model[7] was used to calculate the

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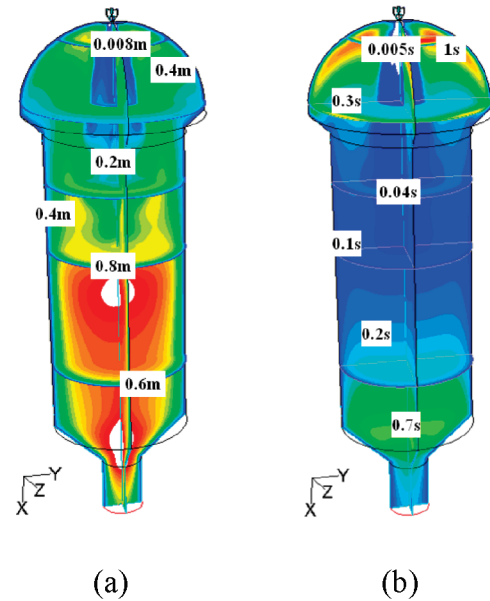
Figure 1. Characteristic (a) length and (b) time scale profiles of integral scale eddies (large eddies).
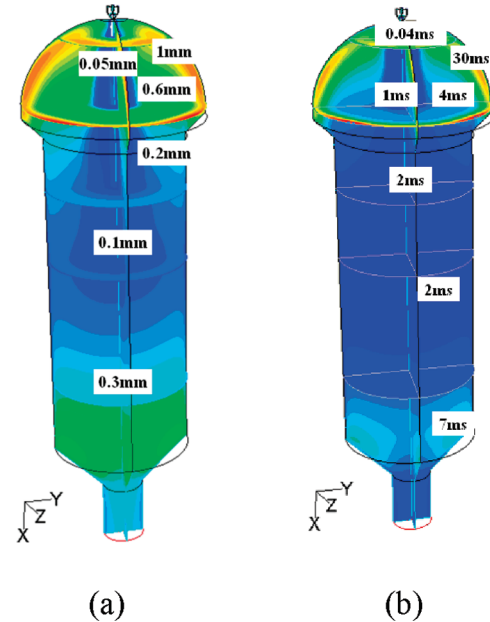

Figure 2. Contours of the (a) length and (b) time scale profiles of Kolmogorov scale eddies (molecular scale).

turbulence information. Coal slurry particles were tracked with the Lagrangian method. The coal slurry gasification process was assumed to be composed by droplet evaporation and the boiling process, devolatilization process, and heterogeneous reactions of coal char particles. The particle-source-in-cell method was used to counter the gas−particle interactions. With this methodology, performance of a 500 tons/day GE gasifier located in Huainan city in China was predicted. The simulation domain was one-quarter of the gasifier, which was represented by a set of $16 \times 32 \times 130$ body-fitted hexahedral meshes. All of the simulation works were completed by the commercial computational fluid dynamics (CFD) software Fluent. The detailed introduction of the simulation can be found in previous work.

On the basis of the simulation and the equations listed in Table 1, the distributions of the characteristic time/length of the integral and Kolmogorov scales are shown in Figures 1 and 2,

Table 2. Reaction Rates of Typical Homogeneous Reactions and Coal Devolatilization in the Gasification Process

reaction	R_i (kmol m^{-3} s^{-1})	A	E (J K^{-1} mol^{-1})	reference
$CO + 1/2 O_2 \rightarrow CO_2$	$R = k_{CO}[CO]^{1.5}[O_2]^{0.25}$	3.16×10^{12}	1.67×10^8	9
$H_2 + 1/2 O_2 \rightarrow H_2O$	$R = k_{H_2}[H_2]^{1/2}[O_2]^{9/4}[H_2O]^{-1}T^{-1}$	2.50×10^{16}	1.67×10^8	10
$CO + H_2O \leftrightarrow CO_2 + H_2$	$R_1 = k_{shift}[CO][H_2O]$	2.75×10^9	8.36×10^7	10
	$R_2 = k_{rshift}[CO_2][H_2]$	1.00×10^8	6.28×10^7	10
$CH_4 + 1/2 O_2 \leftrightarrow CO + 2H_2$	$R = k_{CH_4}[CH_4]^{1/2}[O_2]^{5/4}$	4.40×10^{11}	1.25×10^8	11
coal devolatilization	$dm_p/dt = -A_v \exp(-E_v/RT_p)(m_p - m_{pc})$	2.1×10^5	3.28×10^7	12

respectively. Because the integral scales are strongly affected by initial conditions and geometries, length scales vary in a large range in the gasifier. In the near-nozzle region, the typical integral length scale is only 8 mm, which is about one magnitude smaller than the nozzle diameter. As the jet develops, the integral length scale increases. The maximum integral length scale appears at the middle of the gasifier, where the plug flow pattern starts. The character length scale profile of the integral scale shows the dimension of turbulent fluctuation in the macro-scale in the gasifier, while the time profile represents the frequency of the turbulent fluctuations in the macro-scale. The highest frequency of the integral fluctuation appears near the nozzle, which reveals the characteristics of the high-speed jet. It also proven that there is a strong mixing process in the near-nozzle region because τ_L is inversely proportional to the local stretch rate. At the end of the jet, where the plug flow starts, although the length scale is large, the time scale increases slowly because the gradient of the local velocity is large. At the near-outlet region and furnace dome, the flow is steady, which can be proven by large length scales and low frequencies of the integral scale.

In comparison to Figure 1, Kolmogorov scales are pretty small. In the near-nozzle region, the typical time and length scales are 0.05 mm and 0.04 ms, separately. In most parts of the gasifier, the typical time and length scales are no more than 0.4 mm and 3 ms. Besides that, the variance of the scale distribution through the gasifier is small, except the scales in the near-nozzle region.

2.3. Characteristic Time Scales of Homo- and Heterogeneous Reactions. The homogeneous reaction process is very complex in a gasifier. It is even impossible to identify all of the species that participate in the gasification reactions. However, the whole reaction system can be represented by several global reactions if we are just concerned with the generation of the main species in a gasifier.[8] As long as the characteristic time scales are known for those global reactions, the typical range of the time scales of the homogeneous reactions will be figured out. In this work, four representative homogeneous global reactions are considered. The parameters of these reactions are listed in Table 2.

The kinetic rates k is given by the Arrhenius equation

$$k = A \exp(-E/RT) \qquad (2)$$

On the basis of a constant temperature assumption, the characteristic time scale for each homogeneous global reaction can be calculated by

$$\tau_h = 1/[A\rho Y_R^n \exp(-E/RT)] \qquad (3)$$

where τ_h is the characteristic time scale for a homogeneous reaction. The meaning of τ_h is the period that the reactant concentration drops to $1/e$ of its original value based on the initial temperature. In eq 3, ρ is the gas density, Y_R is the mass

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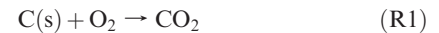
Table 3. A and E for Each Reaction

constant	C + O$_2$[13]	C + CO$_2$[14–16]	C + H$_2$O[17]	C + H$_2$[16]
A (kg m^{-2} s^{-1} Pa^{-n})	300	2224	42.5	1.62
E (J kmol^{-1})	1.3×10^8	2.2×10^8	1.42×10^8	1.5×10^8
n	0.65	0.6	0.4	1

fraction of the Rth reactant, and n is the exponent of the Rth reactant, which are given in Table 2. According to eq 3, the gas temperature has the most important effect on time scales of homogeneous reactions.

Because most devolatilization models are also in Arrhenius form, the characteristic time scale can be identified in the same way. In this work, a one-step devolatilization model was considered. The parameters are listed in Table 2.

Another important process in a gasifier is coal char reactions. Four heterogeneous reactions are considered to represent the char gasification process, which are listed as follows:

$$C(s) + O_2 \rightarrow CO_2 \qquad (R1)$$

$$C(s) = CO_2 \rightarrow 2CO \qquad (R2)$$

$$C(s) + H_2O \rightarrow CO + H_2 \qquad (R3)$$

$$C(s) + 2H_2 \rightarrow CH_4 \qquad (R4)$$

The final reaction rate is determined by the diffusion process and the intrinsic chemical reaction rate and can be calculated by

$$R_i = \frac{R_{i,d} R_{i,k}}{R_{i,d} + R_{i,k}} \qquad (4)$$

where R_i is the final reaction rate of the ith reaction, $R_{i,d}$ is the bulk diffusion rate, and $R_{i,k}$ is the apparent chemical reaction rate. The bulk diffusion rate can be calculated by

$$R_{i,d} = C_i \frac{[(T_p + T_g)/2]^{0.75}}{d_p} p_i \qquad (5)$$

where C_i is the diffusion coefficient of the ith reactant ($C_i = 3 \times 10^{-12}$ s K$^{-0.75}$), T_p is the particle temperature (K), T_g is the temperature of the bulk gas phase (K), d_p is the particle diameter (m), and p_i is the partial pressure of the ith reactant (Pa).

The apparent chemical reaction rate, $R_{i,k}$, is calculated by the nth empirical reaction model, which can be expressed by

$$R_{i,k} = A_i \exp\left(-\frac{E_i}{RT_p}\right)\left(\frac{p_i}{10^5}\right)^n \qquad (6)$$

The pre-exponential A and the activation energy E for each heterogeneous reaction are listed in Table 3.

Similar to the definition of the characteristic time scale of homogeneous reactions, the time scales of each heterogeneous reaction are defined by the period during which coal char particles with a diameter of 70 μm are consumed. For the heterogeneous reactions, it is assumed that the mole concentration of each reactant is kept constant at the typical value in the entrained gasifier and the gas temperature does not change, as well as the particle temperature. Then, the characteristic time scale for the ith heterogeneous reaction, $\tau_{c,i}$, is given by

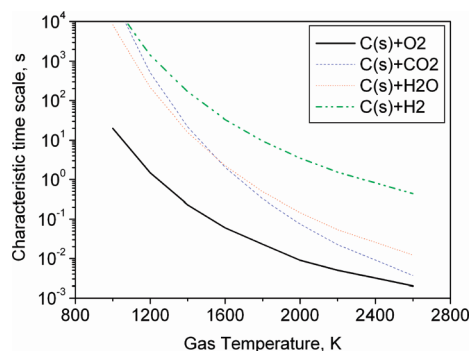$$\tau_{c,i} = m_p/(A_p R_i) \qquad (7)$$

Figure 3. Characteristic time scale profile of each heterogeneous reaction changing with the gas temperature.

where m_p is the char mass in the particle and A_p is the surface area of the particle. On the basis of eq 7, The profiles of $\tau_{c,i}$ changing with the gas temperature are shown in Figure 3. For the char combustion reaction with O_2, there are two inflections as the temperature changes. The first point appears at 1200 K. The whole reaction rate is limited by chemical kinetics when the temperature is lower than this point. The second point appears at 2000 K. The final reaction rate will be limited by the diffusion process when the temperature is larger than 2000 K. When the gas temperature is between these two inflections, the final reaction rate is controlled by both kinetics and the diffusion process.[13,18] For the char gasification reactions, the reaction rates are limited by kinetics in most regions of the gasifier.

3. Controlling Mechanisms in Flame and Nonflame Regions

3.1. Different Regions in the Entrained Flow Coal Gasifier. Wen and Chuang[1] and Smoot and Brown[3] had discussed the characteristics of different regions in the entrained flow coal gasifier. Following their thoughts, the gasifier is divided into three regions: the near-nozzle region, the back-flow region, and the plug-flow region. To have a detailed study on the characteristics of these regions, the numerical results of an entrained flow coal gasifier are discussed and shown in Figure 4. As in Figure 4a, the temperature in the near-nozzle region is pretty high. However, beyond this region, the temperature changes smoothly in a small range. The minimum temperature appears at the dome region, which is about 1400 K. Figure 4b shows the axial velocity profile in the gasifier. The jet speed in the near-nozzle region is more than 50 m/s. Then, the velocity drops to no more than 4 m/s in a short distance. In the back-flow and plug-flow regions, the axial velocity magnitude is no more than 10 m/s. Figure 4c shows the value of $\ln(S_m + 1 \times 10^{-15})$ in the gasifier, where S_m is the particle mass source term (kg/s). As coal particles are injected into the gasifier, the evaporation and devolatilization processes occur rapidly in the

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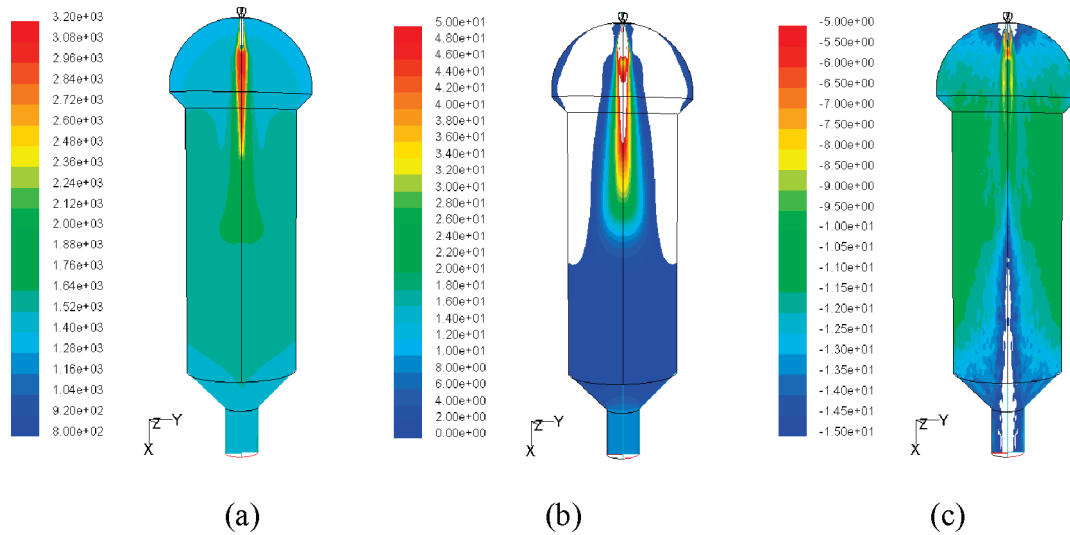
near-nozzle region, which makes most of the mass source yield in the near-nozzle region. In both the back-flow and plug-flow regions, the mass source term of the coal particles is very low.

According to Figure 4, there is no big difference between the back-flow and plug-flow regions except for the flow field. In addition, Figures 1 and 2 also show that the mixing scales in these two regions are in the same magnitude and larger than the scales in the near-nozzle region. In addition, it is enough to divide the gasifier into two regions: the flame and nonflame regions. In the near-nozzle region or flame region, both the temperature and velocity are very high. The gradient is large at the edge of the flame region. In addition, there is also a strong mixing rate. Outside this region or nonflame region, the temperature and species profile change smoothly, the fluctuations are slow, and the length scale is large.

3.2. Scales in the Flame and Nonflame Regions. In the flame region, the typical temperature is set to 2300 K. The characteristic time scales of the homo- and heterogeneous reactions are identified by eqs 3 and 7. The time and length scales of turbulent mixing and particle motion can be identified by numerical simulation. All of the typical time and length scales in the flame region are known and shown in Figure 5. Because the temperature in the flame region is very high, the time scales of heterogeneous reactions and large eddies are in the same magnitude, which means that the turbulent fluctuations in the macro-scale would have a strong effect on the heterogeneous reactions in this region. In the micro-scale flow field, the Kolmogorov time scales are very close to the characteristic time scales of the coal devolatilizaiton process. At the same time, the Kolmogorov length scales are as low as the particle size. This comparison shows that, although the high-speed devolatilization process is not affect by the fluctuation of large-scale eddies, the combustion of the volatile will be affected strongly by the micro-scale fluctuations because the diffusion layer around the particle size will be destroyed by L_η and its fluctuation τ_η. In the combustion region, the oxygen concentration is still at a high level and the homogeneous reactions are dominated by combustion of CH_4, CO, H_2, etc. The time scales of these reactions are much faster than any turbulent fluctuations. Thus, the reactions of the gas phase are controlled by the turbulent mixing process.

In the nonflame region, the typical temperature of the entrained flow gasifier is set to 1600 K. On the basis of this temperature, the time and length scales of each process are shown as Figure 6. Because the devolatilization process has almost completed in the flame region. The time scales of the devolatilization process can be omitted in this region. The time scales of all combustion reactions can also be neglected according to the low oxygen concentration. The important processes in this region are heterogeneous reactions of char gasification and the water shift reaction. The time scales of heterogeneous gasification reactions are much larger than large-scale fluctuations, which means that the turbulent fluctuation has little effect on the char gasification reactions. As a result, it is safe to take the average value of the gas phase when calculating coal char reactions in the nonflame region. Also, even the time scale of the water shift reaction is lower than the smallest turbulent fluctuations. Turbulent mixing is still the controlling effect for homogeneous reactions. However, τ_η in this region is just a littler larger than the time scales of the water shift reactions, which means that there is still

(a)   (b)   (c)

Figure 4. Contours of the (a) temperature, (b) axial velocity, and (c) particle mass source in an entrained flow gasifier.

Figure 5. Typical time and length scales in the flame region.
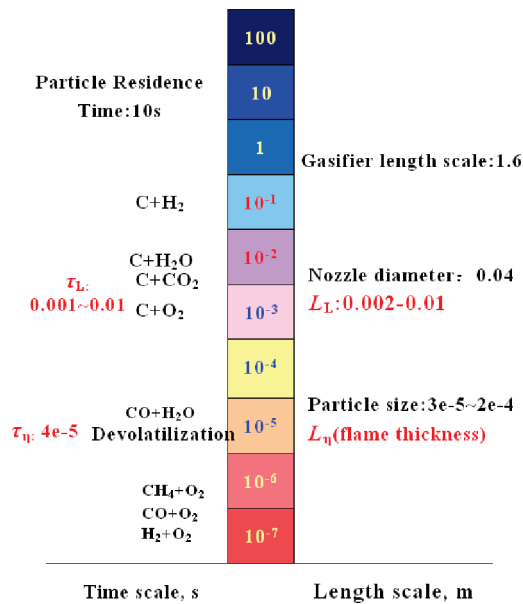

Figure 6. Typical time and length scales in the nonflame region.

a coupling between the homogeneous reactions and turbulent effects.

In the past 3 decades, almost all comprehensive modeling work on coal gasification are based on RANS equations,[8,19−22] also called the RANS method. In these work, the turbulent effects on gas-phase reactions are modeled. However, it is hard to build models to consider the turbulent effects on heterogeneous reactions and the devolatilization process based on the RANS method. This effect, as discussed in this section, is an essential problem in the flame region.

Conclusion

In this work, a systematic analysis on the turbulent mixing effects and the controlling mechanisms in an entrained flow coal gasifier are studied on the basis of comprehensive numerical simulation and fundamental turbulent theories. The length and time scale distributions of large and small eddies are figured out and compared to the characteristic time of homo- and heterogeneous reactions.

In the flame region, the turbulent fluctuations in the macro-scale have a strong effect on the heterogeneous reactions. Although the high-speed devolatilization process is not affected by the fluctuation of large-scale eddies, the combustion of the volatile will be affected strongly by the micro-scale fluctuations in Kolmogorov scales because the diffusion layer around the particle size will be destroyed by L_η and its fluctuation τ_η. The final gas-phase reactions are controlled by the turbulent mixing process.

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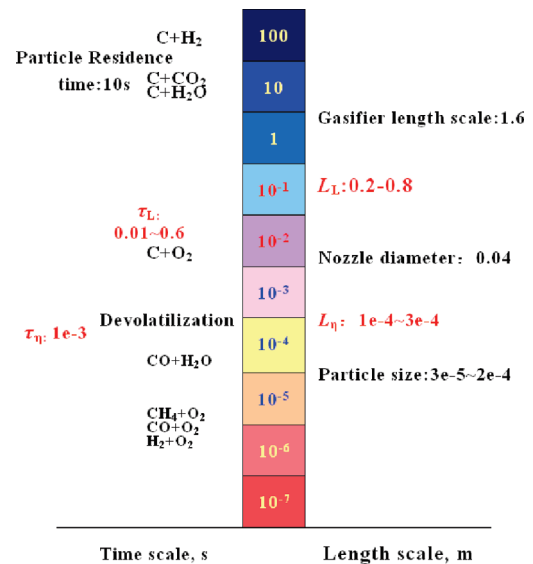
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In the nonflame region, turbulent mixing has little effect on the char gasification reactions. However, coupling between the homogeneous reaction kinetics and turbulent effects should not be omitted.

For a traditional RANS method, it is hard to consider the turbulent effects on particle heterogeneous reactions and the devolatilization process, which makes the simulation in the RANS scheme hard to predict the characteristics of the flame region in an entrained flow coal gasifier.