

Numerical simulation of fluid flow and mixing process in a SCR denitration system

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Abstract. Selective Catalytic Reduction (SCR) with ammonia is a key technology to reduce the NO_x emissions from the coal-fired power stations. The denitration efficiency of SCR system depends on whether the flue gas and ammonia can get a good mix in the reactor. The fluid flow and the mixing process in a SCR denitration system have been analysed to gain an insight into the characteristic of the mixing process and to check the numerical simulation as a tool for the optimization design of the SCR system. Combined with the component transfer model and porous medium model, the large eddy simulation (LES) was carried out to portray the performance of the SCR system in a 310MW coal-fired station. Both the transient and time-averaged velocity fields and concentration fields in different cases were obtained. It has been found that mixing quality is improved significantly by incorporating a series of gate leaves.

1. Introduction

A substantial amount of flue gas including nitrogen oxides NO and NO₂ (collectively called NO_x) is produced in the coal-fired power stations. Atmospheric pollution by NO_x has become a subject of growing concern during the last decades; it is not only are the major contributors to the photochemical smog, but also have direct harmful effects on human health.[1] Therefore, it is important to propose an effective method to control the emission of NO_x in the coal-fired power stations. Based on the work of Srivastava et al.,[2] the technologies of reducing NO_x can be classified into two categories, the primary control technology (PCT) and the secondary control technology (SCT). The PCT uses the staged combustion techniques to reduce NO_x formation in the primary combustion zone. The SCT is used to reduce NO_x in the exhaust gas from the combustion zone, which is also called flue gas denitration (DeNO_x). DeNO_x is further classified into selective nocalytic reduction (SNCR) [3] and selective catalytic reduction (SCR)[4] by whether a catalytic is needed. Due to the selectivity and higher efficiency, the SCR technology is regarded as one of the most important technologies of reducing NO_x.

Optimization of the SCR system to maximize denitration efficiency and to minimize NH₃ slip is one of the main challenges. The SCR system is a complex structure involving several optimization parameter selections, such as the ammonia injection strategy, the instalment of the gate leaf and the hybrid grid, and the thickness and structure of the catalyst layer. [5] Experimental optimizations on an actual SCR system are very difficult, dangerous and expensive. [6, 7] Numerical modelling provides an alternative tool to understand and solve this kind of problem. Most of the reported mathematical models have been performed using the Reynolds averaged Navier-Stokes (RANS) models, such as the *k-ε* or Reynolds stresses.[5,8-12] These models predict time-averaged velocities with reasonable accuracy and at a reasonable computational. However, these models, limited by the RANS's nature, are not suited for modelling the evolution of transient flow pattern triggered by flow instabilities. However, relatively little work has been reported on the transient turbulent flow in the SCR system.



This information may be important for finding some more effective methods to improve the performance of the SCR system.

In this work, the instability and periodicity behaviours of the mixture gas flow in a SCR system of a 310MW coal-fired station are analyzed using the large eddy simulation (LES). Both the transient and time-averaged velocity fields, pressure fields and concentration fields in different cases were obtained.

2. SCR System

The SCR system mainly contains the following parts: main reactor, ammonia injection grid (AIG), gate leaves, straightener and catalyst layers. The roles of the components above have been described in previous works. A schematic of the current 310 MW SCR system is shown in Fig. 1. Flue gas escaped from the outlet of the economizer firstly flows into the main reactor of the SCR system, and then mixes with the ammonia injected by AIG. The mixed gas flows through several parallel gate leaves and the straightener to make the gases mix fully. Then the mixed gas enters the two catalyst layers in a direction normal to the cross section of the catalyst channels and the denitration reaction occurs. The flue gas after the denitration reaction is discharged from the outlet of the SCR reactor and flows into the next procedure.

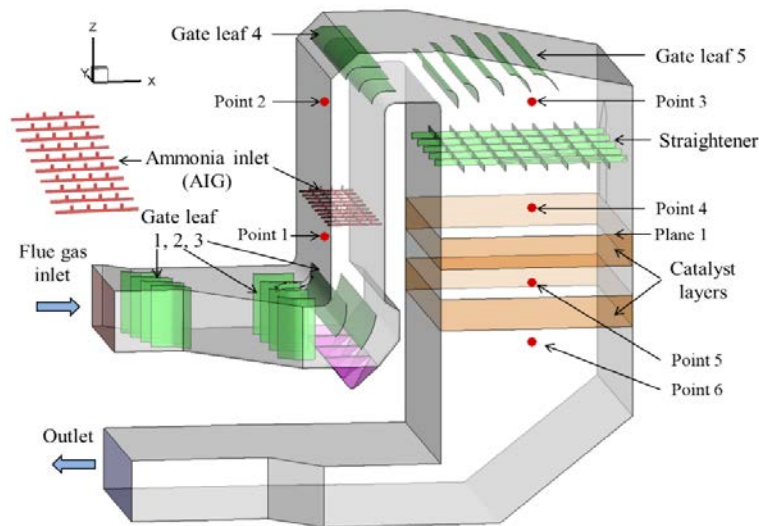
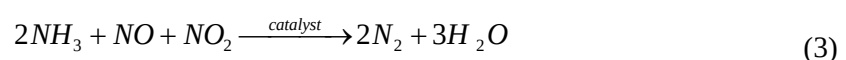
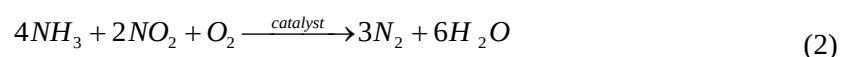
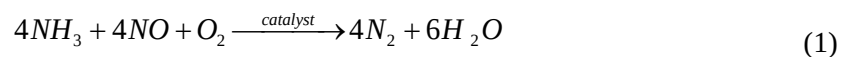


Figure 1. A schematic of the current 310 MW SCR system

Table 1. Flue gas composition injected from the inlet.

	Value		Value
O ₂ (%)	3.3	SO ₂ (ppm) (6% O ₂)	4758
CO (ppm)	110	SO ₃ (ppm) (6% O ₂)	26.33
NO (ppm)	182	N ₂ (%)	73.19
CO ₂ (%)	16.6	Coal ash (g/Nm ³)	46.9

The main chemical reactions for the current SCR system are given below:



Among them, Eq. (1) is the most important reaction since nearly 95% of NO_x exists in the form of NO in the flue gas.

The flue gas composition injected from the inlet into the reactor is shown in Table 1. The total flue gas rate is 624 Nkm³/h. The mass flow rate of NH₃ at the AIG is 67.2 kg/h, and the volume fraction is 5%, the rest is air.

3. Mathematical Model Formation

The aim of the current work is to study the transient flow in the SCR system, some simplifications and assumptions are made as follows:

- (1) Only gas phase flows in the reactor, ignoring the fly ash transport;
- (2) Ignoring the gravity and the chemical reaction in the catalyst layers;
- (3) The catalyst layers are simplified as a kind of porous medium.

Turbulence flow is characterized by eddies with a wide range of length and time scales. The largest eddies are typically comparable in size to the characteristic length of the mean flow. The smallest scales are responsible for the dissipation of turbulence kinetic energy. In the context of LES, the large-scale eddies are resolved directly in the simulation. However, the small-scale eddies are less dependent on the geometry, tend to be more isotropic. So the dissipative effect of the small-scale eddies is represented using a sub-grid scale (SGS) model. The governing equations for transient turbulent flow are generally given as follows: [13]

$$\nabla \cdot (\rho \bar{u}_i) = 0 \quad (4)$$

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial (\bar{u}_i \bar{u}_j)}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left((\nu + \nu_t) \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \right) + S_i \quad (5)$$

where u , t , P , ρ , and ν is velocity, time, pressure, density, and kinematic viscosity. The superscript “ $-$ ” represents filtered. The subscripts i and j represent the three Cartesian directions and repeated subscripts imply summation. The terms on the right-hand side of Eq.(5) are respectively representing the pressure gradient, the stress, and the momentum source term.

The species transport equation can be expressed in the following form:

$$\frac{\partial}{\partial t} (\rho Y_m) + \nabla \cdot (\rho \bar{u}_i Y_m) = \nabla \cdot (D_m \nabla (\rho Y_m)) \quad (6)$$

where Y_m is the mass fraction of the species m , D_m is the diffusion coefficient of the species m in the gas phase.

According to Smagorinsky SGS model, [14] the turbulent viscosity term ν_t is described as follows:

$$\nu_t = L_s^2 |S| \quad (7)$$

where L_s is the mixing length for sub-grid scales, $L_s = \min(k_v d_w, C_s \Delta)$, $\Delta = (\Delta_i \Delta_j \Delta_k)^{1/3}$ is the filter width; S is the characteristic filtered rate of strain,.

The momentum source term (S_i) for the catalyst zone was given as follows:

$$S_i = -\left(\frac{\mu}{\alpha} \bar{u}_i + \frac{1}{2} C_2 \rho |\bar{u}_i| \bar{u}_i \right) \quad (8)$$

where $1/\alpha$ and C_2 are separately the viscous resistance coefficient and inertial resistance coefficient.

4. Numerical Details

Considering the complexity of the geometry, the computational domain was split into several subdomains, which were meshing respectively. Tetrahedral non-structural grids were used in the gate

leaf zones and AIG zone; the other zones were meshed using the hexahedral structured grids. The mesh number in the whole SCR system is about 4.2 million.

The boundary conditions are as follows:

- (1) Flue gas inlet: a uniform velocity of 17.67 m/s, a constant temperature 622.2 K (measured);
- (2) AIG inlet: a uniform velocity of 2.42 m/s, a constant temperature 423 K (measured);
- (3) Outlet: a standard atmospheric pressure;
- (4) Wall: no slip wall, a constant temperature 610 K (assumed).

The computational cost involved with LES is normally orders of magnitudes higher than that for steady RANS calculations in terms of memory and CPU time. In order to save the calculation time, this calculation was first carried out using the standard $k-\epsilon$ turbulence model to obtain a steady flow field. Running until the flow field is reasonably converged and then run LES until the flow becomes statistically steady. The best way to see the fully developed flow and statistically steady is to monitor solution variables (e.g., velocity components) at selected locations in the flow. Additionally, it will help in reducing the time needed for the LES simulation to reach a statistically stable mode. The time step size for LES is 1×10^{-3} s.

5. Results and Discussion

Typical instantaneous velocity fields at different times on the $y=9.2$ m section in the SCR reactor with a series of gate leaves are shown in Figure 2 (a) to (c). It can be seen that the flow is complex and consists of multiple vortices in the SCR reactor, especially around the corner, in which are the locations of the gate leaves. The flow pattern is changing and non-uniformity. The time-averaged velocity field for this reactor is given in Figure 2 (d). Several high velocity zones are found near the gate leaves, indicating that the effect of gate leaves on the flow pattern of flue gas is important. Compared with the result of Figure 2 (e), which is the instantaneous velocity fields in the SCR reactor without any gate leaves, the flow pattern are changed by these gate leaves; the velocity non-uniformity has been improved. However, a big secondary recirculation flow is found around the straightener in the reactor without any gate leaves.

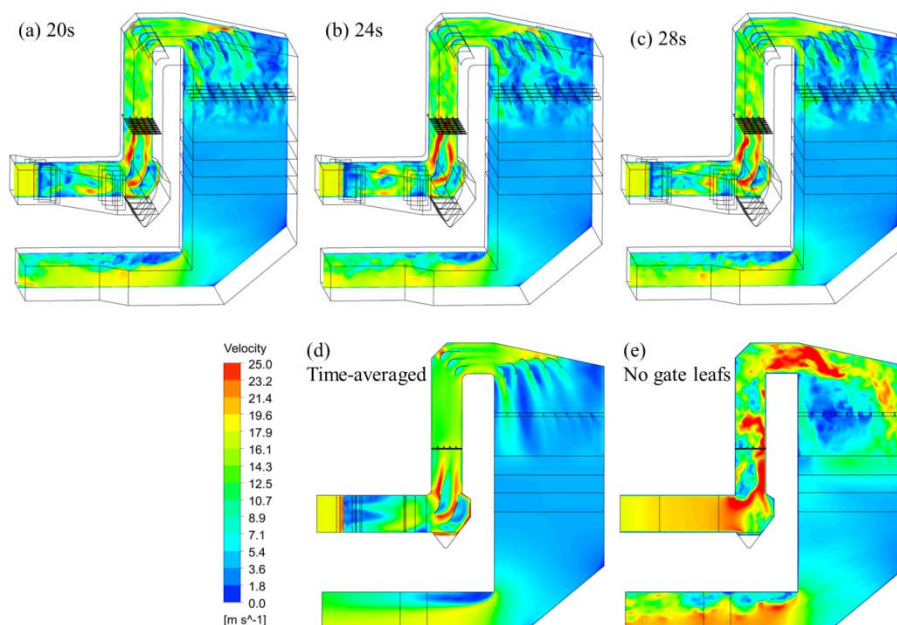


Figure 2. Instantaneous and time-averaged velocity distribution in the $y=9.2$ m section

Figure 3 (a) and (b) respectively show the instantaneous streamlines of flue gas and NH_3 in the SCR reactor at 20s. From the figures we can see that the streamlines of NH_3 are almost the same with of the flue gas. Mixing gas of Flue gas and NH_3 deflects well at the corners of the SCR reactor under the action of inertial force and centrifugal force induced by the gate leaves. The fluid flow is almost

perpendicular to the cross section of the SCR reactor when the mixing gases flow into the catalyst entrance section.

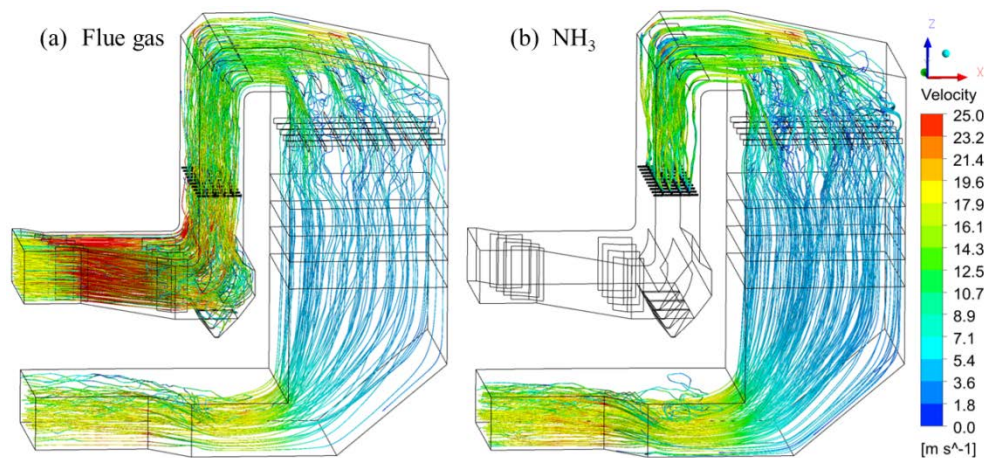


Figure 3. The instantaneous streamlines of flue gas and NH_3 in the reactor

Figure 4(a) to (c) shows the instantaneous simulation results of concentration distributions (NH_3 mass fraction) on plane 1. The NH_3 mass fraction distributions at various times also show that the flow pattern is ever-changing. Figure 4(d) shows the time-averaged NH_3 mass fraction on plane 1. It can be seen that the NH_3 gas flows into the first catalyst layer mainly at central area of the entrance section. Two regions with lower NH_3 mass fraction are found at the two corners on the left of this section.

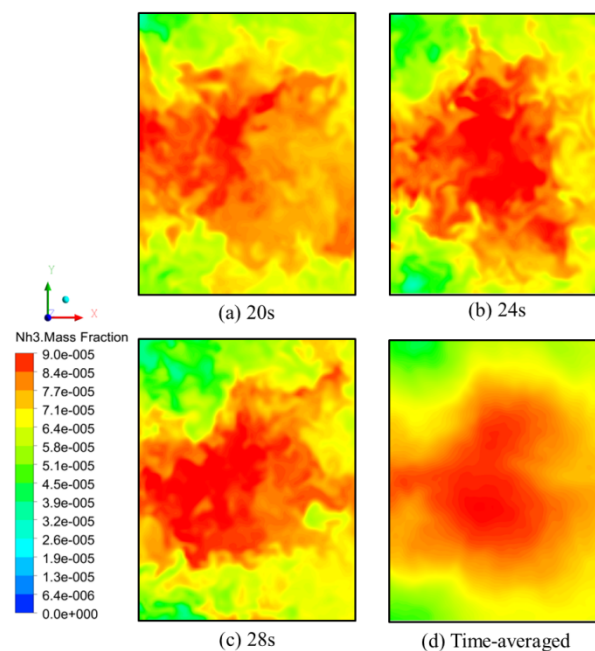


Figure 4. Instantaneous and time-averaged NH_3 mass fraction on the plane 1

A number of researchers [15-17] reported that the fluid flow in any reactor is not stationary but changes over frequently. The periodical behaviour of NH_3 mass fraction in the reactor is identified through some different monitoring points, as shown in Figure 5. The transient values were collected every 0.001 second for 20 seconds. The NH_3 mass fraction distributions show that the flow pattern is ever-changing. This result fully shows that the mixing gases turbulent field in the reactor is transient and random. The flow pattern is changeover (Figure 2), but the time intervals for changeover appeared

to vary randomly. Further study on the transient turbulence mixing flow in the SCR reactor should be considered.

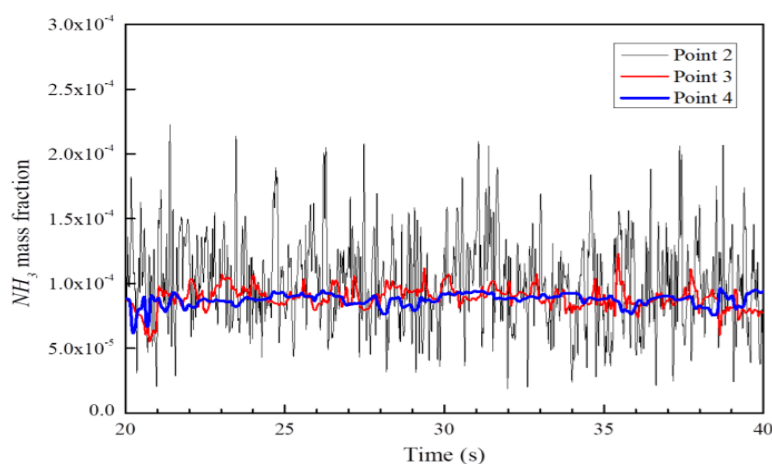


Figure 5. Instantaneous NH₃ mass fraction at different monitoring points

6. Conclusion

The large eddy simulation was carried out to portray the performance of the SCR system in a 310MW coal-fired station. Both the transient and time-averaged velocity fields and concentration fields in different cases were studied. The mixing quality is improved significantly by incorporating a series of gate leaves. The transient turbulence information may be important to the optimization of the SCR reactor structure. Further study on the transient turbulence mixing flow in the SCR reactor should be considered.

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