Study on Pollutant Emission in a Natural Draft Dry Cooling tower with Flue Gas Injection based on LES

Ying Zhou 1, Haihong Xu 2*, Zhen Xu 3, Li Ding 3

1Changzhou Vocational Institute of Mechatronic Technology, Changzhou, China
2Appraisal Center for Environment & Engineering, Ministry of Ecology and Environment, Beijing, China
3State Environmental Protection Key Laboratory of Atmospheric Physical Modeling and Pollution Control, National Environmental Protection Research Institute for Electric Power, Nanjing, China

*Corresponding author e-mail: haihong99@126.com

Abstract. This study investigated the Computational Fluid Dynamics (CFD) simulation of pollutant emission in a natural draft dry cooling tower (NDDCT) with flue gas injection. In order to predict the diffusion and distribution characteristics of the pollutant more accurately, Large Eddy Simulation (LES) was applied to predict the flow field and pollutant concentration field and compared with Reynolds Average Navier-Stokes (RANS). The relationship between pollutant concentration pulsation and velocity pulsation is emphatically analyzed. The results show that the maximum value of LES is about 43 times that of RANS for the prediction of pollutant concentration in the inner shell of cooling tower. Compared with RANS, LES can simulate flow field pulsation with a smaller scale and higher frequency.

Keywords: NDDCT; flue gas; pollutant diffusion; RANS; LES.

1. Introduction
In view of the strict environmental regulations issued by many countries, coal-fired waste gas must be treated by denitrification, dust removal and desulfurization before entering the atmosphere [1]. Limestone wet flue gas desulfurization (FGD) technology has been widely used in coal-fired power plants all over the world for its high efficiency and reliability [2]. After desulfurization, the flue gas temperature can be reduced to about 50 ℃, and the Froude number is not high enough to be discharged into the atmosphere directly. The general method is to reheat the flue gas through a gas-gas heat exchanger (GGH) [3] and then introduce it into the chimney. However, reheaters can complicate the system and increase investment costs. Another method is to introduce low-temperature flue gas into cooling tower and discharge it through the thermal updraft of cooling tower. Nevertheless, it should be noted that the inner shell surface area of cooling towers is much larger than that of traditional chimneys; thus, the cost of corrosion protection will increase greatly. Hence, it is significant to accurately predict the diffusion of flue gas in the cooling tower.

Accurate prediction of pollutant diffusion is one of the hot topics in fluid mechanics. In recent years, numerous published studies focus on flue gas diffusion in coal-fired power plant based on CFD method.
Klimanek et al. [4] found that the increasing wind speed caused the formation of recirculation regions of flue gas flow near the tower outlet increasing the risk of corrosion of tower shell by numerical modeling of NDDCT with flue gas injection. Jahangiri [5] incorporated the flue gas duct in NDDCT modeling and found the flue gas injection with wind breaking wall caused enhancement on the sucked air flow rate and the radiator heat rejection and thus the overall performance under crosswind conditions. Numerical simulation of NDDCT conducted by Eldredge et al. [6] revealed that among various flue gas related variables the flue gas temperature was the key variable affecting tower performance through the buoyancy effects. Schatzmann et al. [7] found that for most cases, such as low wind speed and moderate wind speed, flue gas discharged by cooling tower is better than the traditional chimney; the traditional chimney smoke performs better only in a few strong wind conditions. Yang et al. [8] applied the CFD method to simulate the distribution of pollutants such as gaseous pollutants and particulate matter from flue gas emissions in a coal-fired power plant. The emissions were studied in a natural draft cooling tower with flue gas injection and a chimney. The results indicated that natural draft cooling tower with flue gas injection is more appropriate for flue gas emission than chimney.

Thus far, as shown in the previous literature, most of the studies on numerical simulation of pollutant diffusion in NDDCT with flue gas injection are all based on the RANS model. However, with the improvement of computing power, LES with the capability of better dealing with turbulence fluctuations has become a promising and preferred methodology to simulate various turbulent flow phenomena [9-11]. LES shows better agreement with experimental results than RANS in terms of the distributions of mean velocity and turbulence energy around simple buildings [12-14]. Tominaga and Stathopoulos [15] investigated the flow dynamics and pollutant dispersion in a simple three-dimensional street canyon by comparing RANS (RNG k-ε) and LES, and found that LES yielded better results than RNG k-ε in modeling the distribution of mean concentration by comparison with wind tunnel experiments. Better performance for LES against RNG was also achieved in the representation of turbulent scalar flux when the modeling system extended to a building array with a point source primarily due to the problematic turbulent Schmidt number in RANS model for scalar transport in complex flow fields [16].

A large number of researches show that LES is in better agreement with experimental results because it can predict turbulence fluctuations more accurately. However, literatures on numerical simulation of pollutant diffusion in NDDCT with flue gas injection are all based on RANS model, and there are only a few reports of simulations using LES. In view of this, two models, RANS and LES, are adopted in this paper to simulate the flue gas diffusion for NDDCT with flue gas injection under same working condition. By comparing the differences of equations and flow field characteristics of the two methods, the differences of pollution diffusion characteristics are analyzed. The final results are intended to provide a reference for pollution emissions in the energy industry.

2. Numerical model

2.1. Numerical Approaches

The mathematical equations of RANS and LES are described in many literatures [13][17], only a brief introduction to these two approaches is presented here. Equations 1 and 2 are the momentum equations of RANS and LES, respectively:

\[
\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) = \frac{\partial}{\partial x_j}\left[\mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k}\right) + \frac{\partial p}{\partial x_j} - \frac{\partial}{\partial x_j}(\rho u_i u_j)\right]
\]

\[
\frac{\partial}{\partial t}(\rho \sim u_i) + \frac{\partial}{\partial x_j}(\rho \sim u_i \sim u_j) = \frac{\partial}{\partial x_j}\left[\mu \left(\frac{\partial \sim u_i}{\partial x_j} + \frac{\partial \sim u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial \sim u_k}{\partial x_k}\right) + \frac{\partial \sim p}{\partial x_j} - \frac{\partial}{\partial x_j}(\rho \sim u_i \sim u_j)\right]
\]

The overbar in RANS represents time averaging, and the wavy line in LES represents filtering. The idea of RANS is to average the Navier-Stokes (NS) equation and transform the unsteady turbulence problem into a steady problem, at the cost of an additional unknown, called Reynolds stress, which is
in Equation 1. The idea of LES is to filter the NS equation, use a direct numerical simulation for
large scale turbulence, and describe the turbulence smaller than the filter scale with some model.
Mathematically, turbulence smaller than the filter scale is represented by an additional stress term called
subgrid-scale stress, which is \( \rho \overline{u_i u_j} - \rho \overline{u_i} \overline{u_j} \) in Equation 2. On the surface, the two equations look very
similar. However, LES can still simulate unsteady turbulence essentially, but at a much wider scale.
However, RANS abandoned the simulation of unsteady turbulence information and only sought the flow
results in the average sense. The two approaches start from completely different points of view.

In RANS simulations, the Realizable k-\( \varepsilon \) [18] was employed, and the standard Smagorinsky model
[17] was used for the sub-grid scale eddy viscosity model in LES simulations. Descriptions of Realizable
k-\( \varepsilon \) and LES approaches have been mentioned in many literatures [14], [19], which will not be repeated
here. Transient computation is necessary for LES model, and the time step was set to 0.1 s. To remove
the influence of initial conditions, 500 s (5000 time steps) was firstly promoted to reach a relatively
stable state. Then, time averaging was conducted for 1000 s to obtain statistical values, and it was
confirmed that the statistical values remain unchanged over time. The pressure-based segregated
algorithm Semi-Implicit Method for Pressure Linked Equations (SIMPLE) was used to deal with
pressure and velocity. The second order upwind method was applied to discretize the momentum,
turbulent and energy equations. For LES simulation, the bounded central differencing method was used
to discretize the momentum equation. Convergence was assumed when the scaled residuals drop to the
order of 10-5 or the monitored variables (mass-weighted average temperature at the exit plane of the
cooling tower outlet and the air mass flow rate of the cooling tower) remained stable [19].

2.2. Geometry
A natural draft dry cooling system equipped with FGD system was taken into consideration. The FGD
system is laid out in the center of the natural draft dry-cooling tower and simplified to a cylinder with
the height of 56 m and diameter of 9 m, the main dimensions of cooling tower as well as the FGD system
are shown in Figure 1. The computational domain of this model is illustrated in Figure 2, where the
types of the boundary conditions applied at the outer boundaries are indicated and the computational
domain is large enough to eliminate the unrealistic effect of the domain boundaries on the flow field.

![Figure 1. Main dimensions of cooling tower.](image1)

2.3. Mesh
The quality of the mesh plays a significant role in the accuracy and stability of the numerical
computation. The computational mesh shown in Figure 3 is composed of 8.02 million hexahedral cells
and prismatic cells.
2.4. Boundary conditions

The ground and the surface of the cooling tower were assumed to be no-slip and adiabatic boundary conditions. The boundary conditions at the leeside and top of the computational area were the pressure outlet; the boundary condition of windward side was the velocity inlet, with the form defined as:

\[ U(z) = U_r \left( \frac{z}{10} \right)^\alpha, \]  

(3)

Where \( z \) is height. In this study, \( U_r = 4 \) m/s was the velocity at the referred height (10 m), and the wind profile index \( \alpha \) was assumed as a typical value of 0.2. The turbulent kinetic energy \( k \) and the turbulent dissipation rate \( \varepsilon \) were set following the guidelines provide by Tominaga et al. [20] in both Realizable \( k-\varepsilon \) and LES. The vortex method was adopted for generating the fluctuating inlet boundary in LES, and the number of vortexes was the default value of 190.

The heat exchanger bundles were the heat source and the main source of resistance for the cooling tower, but the size of heat exchanger bundles was so small that it is almost impossible to fully simulate the details [21]. In this study, the heat exchanger bundles were simplified into the radiator model. The pressure drop \( \Delta p \) across radiator was defined in the form:

\[ \Delta p = k_L \frac{1}{2} \rho v^2, \]  

(4)

Where \( \rho \) is the air density, \( v \) is the airflow velocity in the normal direction of the radiator, and \( k_L \) is the non-dimensional loss coefficient, defined as:

\[ k_L = \frac{1}{v} \sum_{n=0}^{N} r_n v^n, \]  

(5)

Where \( N \) is set to 2 and \( r_n \) are polynomial coefficients defined as \( r_0 = 48.675, r_1 = -6.305, r_2 = 0.299 \). The heat transferred to the air by the radiator is obtained by the following equation:

\[ q = h \left( T_{ext} - T_{air,d} \right), \]  

(6)

Where \( T_{ext} \) and \( T_{air,d} \) are the temperature of the radiator and the air downstream of the radiator, respectively. \( h \) is the convective heat transfer coefficient, defined as:

\[ h = \sum_{n=0}^{N} h_n v^n, \]  

(7)

Where \( N \) is set to 2 likewise, \( h_0, h_1, \) and \( h_2 \) are set to 17,683.43, -9167.38, and 1938.02, respectively. It should be noted that the purpose of this paper was to compare the performance of RANS and LES in
pollutant diffusion simulation transversely, thus, the relevant parameters did not need to be very accurate, as long as they were within a reasonable range.

The real flue gas contains SO2, NOx, CO2, etc. SO2 was only simulated, since no chemical reactions were considered in this study. Thanks to ultra-low emission transformation, the average SO2 emission concentration of the large coal-fired units of the China Energy Investment Corporation was about 20 mg/Nm3 (approximately equal to 7 ppm). The boundary condition of flue gas injection outlet was set as the mass flow rate with a value of 929.753 kg/s, and the temperature of flue gas was set to 50 ℃. It was assumed that the parameters of the injected flue gas are the same in all of the cases.

3. Model Validation
Since limited field measurements of NDDCT with flue gas injection were available, the constructed model was validated against recently published relevant data on the heat transfer in NDDCT and pollution dispersion in street canyon in the following procedure. The computational accuracy of CFD method in heat transfer of NDDCT was firstly verified by comparison with the results by Li et al. [19], and then the simulation ability of pollutant diffusion was verified against experimental and simulation data by Tominaga et al. [15]. Figure 4 shows the comparisons of the simulation and literature results. In Figure 4 (a), the simulated results are in good agreement with those in the reference. In Figure 4 (b), there are some differences between the simulation results in this paper and those in the reference, which may be due to the differences in the definition of computational domain and mesh generation between this paper and references. However, the trend of the two results is basically the same, and the high accuracy of LES is also reflected. This conveys that the numerical model has a good computational accuracy in the simulation of both heat transfer and pollution dispersion and can be used for further study.

![Figure 4](image-url)  
**Figure 4.** Numerical model validations: (a) heat transfer validation with Li et al. [19] and (b) pollutant dispersion validation with experiment results [15].

4. Results and discussion

4.1. Performances
Figure 5 shows the time evolutions of air mass flow rate and heat rejection of cooling tower by RANS and LES. It can be seen that the air mass flow rate and heat rejection of cooling tower obtained by RANS were slightly higher than those obtained by LES, and the fluctuation of RANS was very small compared with LES. Both RANS and LES showed a highly similar trend of mass flow and heat dissipation over time.
Figure 5. Time history curves of cooling tower performances: (a) mass flow rate and (b) heat rejection.

Discrete Fourier Transform (DFT) can be used to obtain the amplitude spectrum of any signal that changes with time. Taking mass flow rate as an example, the amplitude spectrum after DFT is shown in Figure 6. It should be noted that the amplitude spectrum here has filtered out the dc part (i.e., the signal with a frequency of 0). Firstly, it can be seen that the maximum amplitude value in the amplitude spectrum of RANS simulation results was much smaller than LES. Secondly, with an increase of frequency for RANS, the amplitude decreases monotonically, while the frequency with the largest contribution in LES was the sub-low frequency 0.00244 Hz. The airflow through the cooling tower was directly related to its internal and external velocity distribution. The mass flow rate of RANS fluctuated very little, which means that the flow field obtained by RANS simulation was very stable and close to a steady flow. However, the mass flow rate of LES fluctuated greatly, indicating that LES can capture the unsteady information that cannot be obtained by RANS.

Figure 6. Comparison of mass flow rate amplitude spectrum.

4.2. Flow field

Figure 7 shows that both two methods can simulate the separation at the inner wall near the radiator and the lee side of the cooling tower. However, the leeward speed ranges of cooling tower in RANS were significantly smaller than that in LES, which will affect the air mass flow rate of the downwind radiator. The difference of velocity distribution explains the diversity of mass flow rate between RANS and LES in the previous subsection. The velocity near the outlet of cooling tower was greater than that of LES, indicating that the mixture of flue gas and hot air was more sufficient in LES. This is because LES was far more capable of capturing unsteady flow than RANS, and turbulence can enhance mass and momentum exchange between different flows.
Figure 7. Comparisons of velocity magnitude distribution at vertical plane (y = 0 m) in NDDCT with flue gas injection: (a) RANS; (b) LES.

Vorticity can reflect the disturbance degree of the flow field to some extent, and the disturbance degree of the flow field affected the mass and energy transfer in the flow field directly. Figure 8 shows the comparison of instantaneous vorticity for the two methods in the vertical plane. It can be clearly seen that LES simulated a lot of whirlpools, both inside and outside the cooling tower compared with RANS. RANS can only roughly simulate the velocity shear of flue gas and hot air and the separation flow above the radiator inside the cooling tower. LES could not only simulate the separation of upwind inside, bottom and downwind outside the cooling tower, but also capture the whirlpool generated by the velocity shear between flue gas and hot air. This explains the differences among the speed, pressure, and temperature of the three methods.

Figure 8. Comparisons of instantaneous vorticity magnitude distribution at vertical plane (y = 0 m) in NDDCT with flue gas injection: (a) RANS; (b) LES.

4.3. Pollutant concentration

Figure 9 shows the concentration distribution of pollutants inside the cooling tower. The diffusion of pollutants is essentially heat and mass transfer, and its diffusion characteristics are determined by velocity and temperature distribution. The velocity distribution determines the macroscopic convective motion while the temperature distribution determines the microscopic molecular thermal motion. The distribution of temperature is closely related to the distribution of velocity, thus, in the final analysis, the distribution of velocity field had the greatest influence on the concentration field of pollutants. Velocity can be divided into average velocity and pulsating velocity superposition. The airflow movement is similar to the pipeline flow inside the cooling tower. Due to the same working conditions, the average velocity in RANS, and LES was basically the same, thus, the pulsation velocity becomes the key to affect the pollutant propagation. Limited by the wall surface of cooling tower, the unsteady
information obtained by RANS was very little. On the contrary, LES could not only simulate pulsation velocity with large scale and low frequency, but also capture pulsation with small scale and high frequency. Therefore, the diffusion of pollutants in LES was the most intense, with the lowest concentration of pollutants and the widest range. Figure 10 shows the root-mean-square error (RMSE) of pollutant concentration calculated by RANS and LES. It is obvious that the pulsation amount in LES was much larger than that in RANS. This not only verifies that flow field pulsation has a great impact on pollutant diffusion, but also reflects that RANS lags far behind LES in capturing unsteady information.

![Figure 9](image1.png)

**Figure 9.** Comparisons of the pollutant concentration distribution at vertical plane (y = 0 m) of cooling tower: (a) RANS; (b) LES.

![Figure 10](image2.png)

**Figure 10.** Comparisons of the root-mean-square error (RMSE) pollutant concentration distribution at vertical plane (y = 0 m) of cooling tower: (a) RANS and (b) LES.

Under the influence of ambient wind, the pollutant tended to approach the wall in the downwind direction of cooling tower. Once the flue gas touched the cooling tower wall, the risk of cooling tower wall corrosion was greatly increased. Figure 11 shows the pollutant concentration in the inner shell of cooling tower simulated by the two methods. For the convenience of observation, the 3D cooling tower inner shell surface was projected onto a two-dimensional (2D) plane. It can be seen that the results of LES were far better than those of RANS in terms of maximum value and range. In RANS, the maximum concentration of flue gas at the cooling tower inner wall surface was 0.0012 ppm, and the influence range of flue gas on the inner wall of cooling tower was roughly above throat and 1/4 downwind. The maximum pollutant concentration in LES was 0.052 ppm, about 43 times that of RANS. The influence range in LES was approximately above 120 m downwind area, which was about 3–4 times of RANS. It can be seen that the result obtained by RANS is much more conservative than LES in the prediction of pollutants at the cooling tower inner wall surface.
5. Conclusion
The flow around NDDCT with flue gas injection is a complex three-dimensional unsteady flow problem. The air mass flow rate and heat rejection of the cooling tower predicted by RANS may meet the engineering accuracy requirement. However, in terms of pollutant diffusion simulation, results obtained by RANS are still not ideal even if the unsteady algorithm is adopted. The flow field will be disturbed by the pulsation, which will affect the distribution of pollutants. When used to simulate the NDDCT with flue gas injection, LES is capable of capturing details and pulsations of flow field that RANS cannot capture. Therefore, LES is necessary to accurately simulate pollutant diffusion in the future, especially the organized pollution sources of thermal power enterprises in the energy industry.

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