Influence of turbulence boundary condition on pollutant diffusion for a natural draft cooling tower with flue gas injection

Guangjun Yang 1,2, Li Ding 2 and Zhaobing Guo 1,*

1 School of Atmospheric Physics, Nanjing University of Information Science & Technology, Nanjing, China
2 State 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: guozbnuist@163.com

Abstract. The influence of the specification of turbulence model in equilibrium atmosphere boundary layer (ABL) on the numerical simulation of pollutant diffusion for a natural draft cooling tower with flue gas injection is investigated. The ABL must be considered due to the immense size of cooling tower. The flow field and pollutant distribution under the circumstance of different turbulence boundary conditions are predicted by solving Navier-Stokes (N-S) equations based on shear-stress transport (SST) $k$-$\omega$ turbulence model. The results indicate that the pollutant distribution remains almost unchanged when the turbulence boundary condition changed, it can be inferred that the turbulence boundary condition has little effect on the diffusion of pollutant for other Reynolds Average Navier-Stokes (RANS) turbulence models. Since RANS cannot consider the fluctuation velocity, it is not very suitable for predicting the pollutant diffusion. To more accurately simulate the pollutant propagation and diffusion, the large eddy simulation (LES) model is needed.

Keywords: equilibrium ABL; pollutant diffusion; natural draft cooling tower; flue gas injection; SST $k$-$\omega$; RANS.

1. Introduction

In consideration of the cooling tower can reach height of 200m or more, numerical simulation of cooling tower with flue gas diffusion is a typical computational wind engineering (CWE) problem and the wind profile of the ABL must be considered. The modeling of equilibrium ABL is an important precondition for numerical simulation of flows around buildings. The horizontal inhomogeneity of the simulated ABL will result in additional errors to numerical results, and sometimes the influences of the additional errors are significant [1]. Richards et al.[2] emphasized the requirements of modeling of an equilibrium ABL for the numerical investigation of flow around buildings. Blocken et al.[3] pointed that CFD simulation of a horizontally homogeneous atmospheric boundary layer flow was difficult and it was vital for the successful application of CFD in wind engineering studies. Hargreaves and Wright [4] model the ABL
by using k-ε model, they found the neutral ABL can be maintained along a lengthy fetch but only with a modified law of the wall and with a shear stress applied to the top boundary of the domain.

With the development of economy and urbanization, problem of air pollution becomes more and more serious. As an important part of the industrial system, large amount of waste gases such as sulfur dioxide and oxynitride are discharged into the atmosphere from coal-fired power plants every year. In recent years, numerous studies focus on flue gas diffusion in coal-fired power plant based on computational fluid dynamics (CFD) method have been published. Klimanek et al.[5] presented a study on numerical modeling of a natural draft wet-cooling tower with flue gas. It is concluded that the increasing wind speed is a reason of recirculation regions formation near the tower outlet which leads to flue gas flow near the tower shell increasing the risk of corrosion. Schatzmann et al.[6] compared the ground-level concentrations produced by the cooling tower discharge method and those produced by a traditional stack. It was found that for low and intermediate wind speeds, the ground level concentrations are lower for the case of the cooling tower discharge. Only for strong winds, which occur only very rarely at most German sites, did the conventional stack discharge appear to be superior.

However, in most studies about flue gas diffusion, the modeling of equilibrium ABL was neglected, which means only velocity profile was considered but turbulence profile was ignored. The main objective of this study is to investigate the influence of equilibrium ABL on flue gas diffusion, especially the influence of turbulent boundary conditions on pollutant diffusion.

2. Numerical model

2.1. 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)

![Figure 2. Computational field.](image2)

2.2. 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 was generated by using ANSYS ICEM CFD and is composed of 8.02 million hexahedral cells and prismy cells.
2.3. Operating conditions
The gravitational acceleration was specified as 9.8 m/s\(^2\). The reference pressure location was put at a point 2000 m upstream from the center of the cooling tower at ground level. The operating pressure, temperature and density are 101710 Pa, 15.5 °C and 1.218 kg/m\(^3\) respectively.

3. Equilibrium ABL

3.1. Theory of equilibrium ABL
Tang et al.[7] Derived the inflow boundary conditions for general CWE based on the k-\(\omega\) turbulence model and the assumption of equilibrium turbulence. The suggested inflow turbulence boundary conditions are

\[ k = \frac{C_1}{\alpha} z^\alpha + C_2 \]  
\[ \omega = \frac{\alpha}{\sqrt{\beta}} \frac{U_r}{z_r^\alpha} z^{\alpha-1} \]

Where \( z \) is height, \( k \) and \( \omega \) are turbulence kinetic energy (TKE) and specific dissipation rate respectively, \( z_r \) is the reference height and \( U_r \) is the velocity at \( z_r \), the wind profile index is \( \alpha \), \( \beta \) is a constant set as 0.0001.

\( C_1 \) and \( C_2 \) are two adjustable parameters, and some assumptions must be made before estimating their value. In ABL, the turbulence is assumed to be isotropic [8], the TKE is defined as

\[ k = \frac{3}{2} [U(z)^* I(z)]^2 \]

Where \( U \) is the magnitude of velocity, \( I \) is the turbulence intensity.

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

\[ I(z) = 0.1 \left( \frac{z}{z_G} \right)^{-\alpha-0.05} \]

Where \( z_G \) is the gradient wind height. \( k \) in equation (7) can be determined by equations (8) and (9), then \( C_1 \) and \( C_2 \) can be solved according to the results in equation (7) based on least square fit method.
3.2. Modeling of equilibrium ABL
Before simulating the flow of cooling tower, a 2-D numerical model of empty domain with no obstacle is built firstly, in which the calculation domain is set as 2000 m (H) × 6000 m (L) as shown in Figure 4. The wind profile index is set as 0.2, velocity at height of 10m is 4 m/s.

![Figure 4. Mesh of the 2-D numerical model.](image)

After the numerical iterations converged, the velocity and the TKE profiles along the four locations, inlet face, 1/3L (L is the length of the domain), 2/3L and the outlet face are compared respectively and presented in Figure 5. The wind profiles almost completely coincide, and the basic characteristics of the ABL remain ideal even after flowing through the computational domain space with a length of 6000 m, it provides confidence for the subsequent research by using this method.

![Figure 5. Mean velocity and TKE profiles of simulated boundary layer.](image)

4. Results and discussion
In order to investigate the influence of turbulence boundary condition on pollutant diffusion, four different scenarios as summarized in Table 1 are simulated in all. The velocity profile is same for all scenarios. In Case 1 and Case 3 method for generating equilibrium ABL introduced in Section 3.1 are considered, while the default value of k and ω in Fluent 15.0 are applied in Case 2 and Case 4. In consideration of that the time format may lead to changes in the results, both steady and transient conditions are solved. The time step is set as 0.25s in transient simulations, the results for transient states are obtained by calculating for total 10 minutes on the basis of steady state results that have converged.
**Table 1.** Different boundary condition and calculation settings.

| Name       | Case 1                                      | Case 2                                      | Case 3                                      | Case 4                                      |
|------------|---------------------------------------------|---------------------------------------------|---------------------------------------------|---------------------------------------------|
| Velocity   | $U(z) = 4 \left( \frac{z}{10} \right)^{0.2}$ | $k = \sqrt[0.2]{0.123 - 0.2z^2 + 3.333}$   | $k = \sqrt[0.2]{0.123 - 0.2z^2 + 3.333}$   | 1 (Fluent default)                          |
| $\omega$   | $\omega = \frac{0.2}{\sqrt{0.0001 + 450z^{0.2}}} \cdot z^{0.2-1}$ | 1 (Fluent default)                          | 1 (Fluent default)                          | 1 (Fluent default)                          |
| Time       | Steady                                     | Steady                                     | Transient                                   | Transient                                   |

Figure 6 shows the contours of velocity distributions, temperature distributions, TKE distributions and pollution distributions under different conditions. It can be seen that there is a little bit different but not much between the calculation results of steady state and transient state, this indicates that the flow field around the cooling tower is relatively stable.

![Figure 6](image)

**Figure 6.** Comparison of flow field and pollution distributions among four scenarios.

As is well known, there are two main factors influencing pollutant diffusion, molecular diffusion and convective diffusion, molecular diffusion is mainly affected by temperature and convective diffusion is mainly affected by macroscopic velocity. The temperature and velocity distributions between Case 1 and 2 in Figure 6 are almost the same, this determines that the pollutant diffusions under the two conditions are almost the same.

The real velocity is fluctuating as described in LES, it can be decomposed into average velocity and fluctuation velocity, in which the fluctuation velocity is superposed by the fluctuation velocities of countless different frequencies and different power densities. In general, the spatial scale of low-frequency fluctuation velocity is large, while that of high-frequency fluctuation velocity is small. The lower frequency fluctuation velocity has a greater influence on the diffusion of pollutants, while the
higher frequency fluctuation velocity has a smaller influence on the diffusion of pollutants. In RANS, fluctuation velocity is only a small quantity in the momentum equation, and there is no concept of spectrum, which can be understood as a fluctuation velocity with extremely high frequency and extremely small spatial scale. Therefore, the turbulence intensity in RANS has little effect on pollutant diffusion.

Gousseau et al. [9] compared and simulated the diffusion patterns of pollutants in urban street canyons by using RANS and LES. LES was observed to produce more accurate and reliable results compared to both RANS approaches, because LES resolves the inherent fluctuations, thus captures the turbulent mixing process in the flow field. Although RANS also can compute for transience, it fails to account for unsteadiness, and hence is not an appropriate replacement for LES.

5. Conclusion
In this study, the influence of turbulence model boundary condition on pollution diffusion for a natural draft cooling tower with flue gas injection is investigated. RANS equations based on SST k-ω turbulence model is applied to simulate the velocity, temperature, TKE field and pollutant distributions, both steady and transient states are solved. The results indicate that the pollutant concentration distribution is independent of the setting of turbulence boundary conditions, this is because the fluctuating velocity is just a small amount as a source term in momentum equation in RANS equations and the independent variable of the momentum equation, velocity, is an averaged value. Hence, it can be inferred that the other RANS methods are also not very suitable for prediction of pollutant diffusion. The large eddy simulation (LES) model will be applied to simulate the pollutant diffusion in the future as a further study.

Acknowledgments
This work was supported by the National Natural Science Foundation of China (grant number 51607058, 11372135).

References
[1] W. Yang, Y. Quan, X. Jin, et al. Influences of equilibrium atmosphere boundary layer and turbulence parameter on wind loads of low-rise buildings, Journal of Wind Engineering, 96 (2008) 2080-2092.
[2] P. Richards, B. Younis. Comments on ‘Prediction of wind-generated pressure distribution around buildings’ by Mathews E H, Journal of Wind Engineering and Industrial Aerodynamics, 1990, 34(1) 107-110.
[3] B. Blocken, J. Carmeliet, T. Stathopoulos. CFD evaluation of wind speed conditions in passages between parallel buildings—effect of wall-function roughness modifications for the atmospheric boundary layer flow, Journal of Wind Engineering and Industrial Aerodynamics, 2007, 95(9-11): 941-962.
[4] D. Hargreaves, N. Wright. On the use of the k-ε model in commercial CFD software to model the neutral atmospheric boundary layer, Journal of Wind Engineering and Industrial Aerodynamics, 2007, 95(5): 355—369.
[5] A. Klimanek, M. Cedzich, R. Bialecki. 3D CFD modeling of natural draft wet-cooling tower with flue gas injection, Applied Thermal Engineering, 2015, 91: 824-833.
[6] M. Schatzmann, A. Lohmeyer, G. Ortner. Flue gas discharge from cooling towers. Wind tunnel investigation of building downwash effects on ground-level concentrations, Atmospheric Environment, 1987, 21(8): 1713-1724.
[7] Y. Tang, S. Zheng, B. Zhao, et al. Numerical investigation of the self-sustaining of equilibrium atmosphere boundary layers, Engineering mechanics, 2014, 31(10): 129-135.
[8] B. Huang, C. Wang. Theory and application on structure wind resistant, 2nd Edition, Shanghai: Tongji University Press, 2008: 349.
[9] P. Gousseau, B. Blocken, T. Stathopoulos, et al. CFD simulation of near-field pollutant dispersion on a high-resolution grid: a case study by LES and RANS for a building group in downtown Montreal. Atmospheric Environment, 2011, 45: 428-438.