Evaluation of RSM for Simulating Dispersion of CO\textsubscript{2} Cloud in Flat and Urban Terrains

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ABSTRACT

Accurate and reliable computational fluid dynamics (CFD) simulation of pollutant dispersion is essential for protecting human health, and the choice of turbulence model is an important parameter determining the accuracy of simulation results. This paper evaluates the ability of Repons stress model (RSM) to predict dispersion of carbon dioxide (CO\textsubscript{2}) cloud, which is a typical type of heavy gas and similar to some particulate pollutants, in flat and urban terrains. The RSM simulation is conducted with stress-\(\omega\) model, whereas SST \(k-\omega\) two-equation model is selected as the benchmark. The simulation results are compared with the available wind tunnel measurements, and statistical performance indicators are used to obtain a comprehensive and quantitative evaluation of the performances of the two turbulence models. The results reveal that stress-\(\omega\) model exhibits different capacities in flat terrain and urban terrain. Specifically, stress-\(\omega\) model can present better results than SST \(k-\omega\) model in flat terrain, and it performs better in the far-field region than in the near-field region. Although SST \(k-\omega\) model can describe CO\textsubscript{2} dispersion more accurately in urban terrain, the concentration distribution reproduced by stress-\(\omega\) model is still within acceptable range.

Keywords: Flat terrain; Urban terrain; Stress-\(\omega\); SST \(k-\omega\).

INTRODUCTION

Dispersion of pollutant represents a major threat to human health, and the precise prediction of pollutant concentration distribution is a prerequisite for avoiding adverse air quality impacts (Zhang et al., 2011; Dodla et al., 2017; Guttikunda and Jawahar, 2018). Compared with the simple Gaussian and other analytical dispersion models, computational fluid dynamics (CFD) models can provide results of the flow feature in complicated terrain simultaneously and have been widely employed to investigate pollutant dispersion (Gupta and Chan, 2016; Lateb et al., 2016). Lin et al. (2016) studied the effects of street layout and wall heating on pollutant dispersion by CFD simulation. Huang et al. (2017) applied a CFD model to evaluate the impacts of the upstream building height and stack location on the dispersion of pollutant.

However, CFD models need to be established and evaluated correctly to accurately simulate pollutant dispersion. The selection of turbulence model is one of the prerequisites for CFD simulation, as it greatly affects the reproduction of flow field and the prediction of pollutant dispersion. Among the various turbulence models, the two-equation models are the main approach for turbulence modeling of the practical pollutant dispersion. However, these models are based on the isotropic Boussinesq hypothesis (Lane, 2017), which can make these models lack of the ability to predict accurately the complex flow structure along the ground, thus causing the results to be unreliable (Franke et al., 2005; Longo et al., 2017). To avoid the assumption of isotropy, the Reynolds stress model (RSM) can be used, which in theory should perform better than two-equation models. Yet, in some cases, the converged solution is far beyond satisfaction, and the approach cannot yield any notable gains in accuracy (Wang and McNamara, 2006; Tominaga and Stathopoulos, 2013; Peren et al., 2015). For instance, Sklavounos and Rigas (2004) evaluated four turbulence models (i.e., standard \(k-\varepsilon\) model, standard \(k-\omega\) model, SST \(k-\omega\) model, and Speziale-Sarkar-Gatski (SSG) RSM) against Thorny Island field trials data, and found that SSG model prolonged calculation time with only constrained gains in accuracy. Bartzanas et al. (2007) tested four turbulence models (i.e., standard \(k-\varepsilon\) model, RNG \(k-\varepsilon\) model, realizable \(k-\varepsilon\) model, RSM) for the ventilated airflow, and found that RSM needed long convergence time and showed better performance only under low air velocities.
However, careful inspection of the relevant studies, makes clear that solid conclusion cannot be drawn by simply evaluating the results of the limited number of cases. Therefore, additional research efforts are necessary to further evaluate the performance of RSM in certain cases. In light of this, the present research aims to test the ability of RSM to predict pollutant dispersion in two types of terrains. The first type is the flat terrain, where a relatively simple flow field is observed, while the second is the urban terrain, where the complicated flow structure is produced mainly due to geometric effects (Carpentieri et al., 2015).

SST k-ω model is characterized by an advanced near-wall treatment, taking advantages of both the k-ε and k-ω models. It gets rid of the drawback of the standard k-ε model that unable to describe the near-wall zone, the drawback of the modified k-ε models that cannot capture information in the wake volume, and the drawback of the k-ω model that be sensitive to free stream (Li et al., 2006; Lateb et al., 2013; Yu and The, 2016). Thus, SST k-ω model is used as the reference point for the comparison of the results. Stress-ω model, one of the RSM type, uses the similar boundary condition for ω (Sharif and Guo, 2007). Thus, both models employ the same mesh densities and near-wall grid sizes, and the results are simply determined by the turbulence models themselves. Numerical simulation of CO₂ cloud dispersion in flat and urban terrains were carried out by means of SST k-ω model and stress-ω model, and the results were tested against the available experimental data obtained from the literatures (Xing et al., 2013; Tan et al., 2018). Also, CO₂ cloud is a typical type of heavy gas, and therefore the results can be conducive to the simulation of some particular pollutants dispersion.

TURBULENCE MODEL

SST k-ω Model

SST k-ω turbulence model is a two-equation eddy-viscosity model based on Boussinesq eddy viscosity assumption, taking both the advantage of k-ω model that performs better in the near-wall region and the advantage of standard k-ε model that is accurate and reliable for the flow outside the boundary layer, with a limiter evaluating the proper transport behavior of turbulent shear stress and a blending function transiting between k-ω model and k-ε model on the basis of the distance to the surface and on the flow variables. It has been proved to be able to predict flow field and pollutant dispersion in the atmosphere nicely (Eca and Hoekstra, 2011; Yu and The, 2016). SST is a good benchmark for higher fidelity models such as RSM, to determine if they can accurately predict the flow field and pollutant dispersion (O’Brien et al., 2018). Equations of the model are presented in the following:

\[
\begin{align*}
\frac{\partial k}{\partial t} + U_j \frac{\partial k}{\partial x_j} &= P_k - \beta' k \omega + \left( v + \sigma_k \nu \right) \frac{\partial k}{\partial x_j} \\
\frac{\partial \omega}{\partial t} + U_j \frac{\partial \omega}{\partial x_j} &= \alpha S^2 - \beta \omega^2 + \frac{\partial}{\partial x_j} \left[ (v + \sigma_\omega \nu) \frac{\partial \omega}{\partial x_j} \right]
\end{align*}
\] (1)

ω-equation

\[
\frac{\partial \omega}{\partial t} + U_j \frac{\partial \omega}{\partial x_j} = \alpha S^2 - \beta \omega^2 + \frac{\partial}{\partial x_j} \left[ (v + \sigma_\omega \nu) \frac{\partial \omega}{\partial x_j} \right] + 2(1 - F_1)\sigma_{\omega^2} \frac{1}{\omega} \frac{\partial \omega}{\partial x_j}
\] (2)

The kinematic eddy viscosity is calculated from

\[
v_j = \frac{a_j k}{\max(a_j, \delta F)}
\] (3)

where \( S \) is the strain rate magnitude.

The closure coefficients and auxiliary relations are given by

\[
P_k = \min \left( r_y \frac{\partial U}{\partial x_j}, 10 \beta' k \omega \right)
\] (5)

\[
F_2 = \tanh \left\{ \max \left( \frac{2 \sqrt{B \omega_y}}{500 \nu}, \frac{500 \nu}{y^2 \omega} \right)^2 \right\}
\] (4)

\[
F_1 = \tanh \left\{ \min \left[ \max \left( \frac{2 \sqrt{B \omega_y}}{500 \nu}, \frac{500 \nu}{y^2 \omega} \right), \frac{4 \sigma_{\omega^2} k}{CD_{\omega \omega}} \right] \right\}^4
\] (6)

\[
CD_{\omega \omega} = \max \left( 2 \rho \sigma_{\omega^2} \frac{1}{\omega} \frac{\partial k}{\partial x_j}, \frac{10^{-10}}{\omega} \right)
\] (7)

The constants are summarized as \( \phi = \phi_1 F_1 + \phi_2 (1 - F_1) \), with \( \phi = \sigma_c, \sigma_{\omega^2}, \alpha, \beta, \alpha_1 = 0.31, \alpha_2 = 0.5, \beta_1 = 3/40, \beta_2 = 0.0828, \beta' = 0.09, \sigma_{\omega^1} = 0.85, \sigma_{\omega^2} = 1, \sigma_{\epsilon} = 0.5, \sigma_{\omega^2} = 0.856. 

Stress-ω Model

RSM (Lauder et al., 1975) resolves directly a transport equation for each term of the Reynolds stress tensor separately using differential equations, taking the anisotropy of turbulence into account and making up for the deficiencies of the Boussinesq approximation. According to the modeling of the pressure-strain and dissipation-rate terms, the CFD-Fluent provides numerous types of RSM. Stress-ω model, a stress-transport model based on the omega equation and Launder-Reece-Rodi (LRR) model (Lauder et al., 1975), is considered in this paper. Stress-ω model is similar to k-ω model, mainly reflected in the transport equation for \( \omega \) and the wall boundary condition for \( \omega \) (Sharif and Guo, 2007). The model equations are expressed as follows:
Stress-equation
\[
\frac{\partial \tau_{ij}}{\partial t} + U_k \frac{\partial \tau_{ij}}{\partial x_k} = -P_{ij} + \frac{2}{3} \beta \omega \delta_k \delta_j - \Pi_{ij} + \frac{\partial}{\partial x_k} \left[ (v + \sigma_j^*) \frac{\partial \tau_{ij}}{\partial x_k} \right] \tag{8}
\]

\omega-equation
\[
\frac{\partial \omega}{\partial t} + U_j \frac{\partial \omega}{\partial x_j} = \alpha \frac{\partial}{\partial x_j} \frac{\partial U_j}{\partial x_j} - \beta \omega^2 + \frac{\partial}{\partial x_j} \left[ (v + \sigma_j^*) \frac{\partial \omega}{\partial x_j} \right] \tag{9}
\]

The pressure-strain correlation is given as
\[
\Pi_{ij} = \beta^* C_1 \omega \left( \tau_{ij} + \frac{2}{3} \beta \omega \delta_j \right) - \tilde{\alpha} \left( P_{ij} - \frac{2}{3} P \delta_j \right) - \beta \left( D_{ij} - \frac{2}{3} P \delta_j \right) - \tilde{\gamma} k \left( S_{ij} - \frac{1}{3} S_{ik} \delta_j \right) \tag{10}
\]

where
\[
P_{ij} = r_{in} \frac{\partial U_i}{\partial x_m} + r_{jm} \frac{\partial U_j}{\partial x_m} \tag{11}
\]

\[
D_{ij} = r_{en} \frac{\partial U_i}{\partial x_j} + r_{jm} \frac{\partial U_m}{\partial x_j} \tag{12}
\]

\[
P = \frac{1}{2} P_{ik} \tag{13}
\]

The closure coefficients are defined as $C_1 = 9/5$, $C_2 = 13/25$, $\alpha = 1/2$, $\sigma^* = 1/2$, $\beta_0 = 9/125$, $F^{\omega*} = 9/100$, $C^{\omega*} = 9/100$, $\beta = 8 + C_2 / 11$, $\tilde{\alpha} = 8 + C_2 / 11$, $\tilde{\gamma} = 8 C_2 / 11$, $\hat{\gamma} = 4 S_{11} - 4 \Omega_{12} - 4 S_{22} / 5$, $f_{\beta} = 1 + 70 \chi_{\omega} / (1 + 80 \chi_{\omega})$, $\chi_{\omega} = S_{ii} / \left( \beta_{\omega}^* \omega \right)^3$, $S_{ij} = 1 / 2 \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right)$, $\Omega_{ij} = 1 / 2 \left( \frac{\partial U_i}{\partial x_j} - \frac{\partial U_j}{\partial x_i} \right)$, $\chi_k = 1 / \omega^2 \frac{\partial \omega}{\partial x_j} \frac{\partial \omega}{\partial x_j}$, $f_{\beta} = 1 + 640 \chi_k^2 / (1 + 400 \chi_k^2)$, $\chi_k \leq 0$, $\chi_k > 0$.

**STATISTICAL MODEL PERFORMANCE EVALUATION METHOD**

Five performance measures (Hanna et al., 2004), including the fractional bias (FB), the geometric mean bias (MG), the normalized mean square error (NMSE), the geometric variance (VG), and the fraction of predictions within a factor of two of observations (FAC2), defined as below, were used to obtain a comprehensive and quantitative evaluation of the performances of these two turbulence models for dispersion of CO2 cloud.

\[
FB = \frac{(C_O - C_P)}{0.5(C_O + C_P)} \tag{14}
\]

\[
MG = \exp \left( \ln C_O - \ln C_P \right) \tag{15}
\]

\[
NMSE = \frac{(C_O - C_P)^2}{C_O C_P} \tag{16}
\]

\[
VG = \exp \left[ \left( \ln C_O - \ln C_P \right)^2 \right] \tag{17}
\]

\[
FAC2 = \text{fraction of data that satisfy } 0.5 \leq C_p / C_o \leq 2.0 \tag{18}
\]

where $C_p$ was model predictions of concentration, $C_o$ was observations of concentration, and $C$ was average over the data set.

According to the literature (Hanna et al., 2004), FB = 0, MG = 1.0, NMSE = 0, VG = 1.0 and FAC2 = 1.0 represent the perfect model, and $-0.3 < FB < 0.3$, $0.7 < MG < 1.3$, NMSE < 4, VG < 1.6 and 0.5 < FAC2 represent the acceptable range.

**EVALUATION OF STRESS-$\omega$ MODEL IN FLAT TERRAIN**

**Description of Wind Tunnel Experiment Considered**

This experiment (Xing et al., 2013) conducted by the Beijing Institute of Technology was simulated, and the simulation results were compared with experimental data to conduct the evaluation of stress-$\omega$ model for simulating dispersion of CO2 cloud in flat terrain. The experiment was implemented in a 6.4-m-wide, 5.2-m-high wind tunnel located in Zhangjiakou. The sonic anemometer was placed at the wind inlet at a height of 2 m to measure the wind speed. In the trials, the CO2 inlet had a radius of 0.01 m and CO2 of 99.9% by volume was oriented vertically upwards under atmospheric pressure, which could realize the simulation of pollutant dispersion from a point release at the ground level (Shen et al., 2017; Wingstedt et al., 2017).

Four different cases with CO2 flow rates of 166.7 L min$^{-1}$, 200 L min$^{-1}$, 250 L min$^{-1}$, 300 L min$^{-1}$, corresponding to the flow speeds of 8.8 m s$^{-1}$, 10.6 m s$^{-1}$, 13.3 m s$^{-1}$ and 15.9 m s$^{-1}$, were carried out. Ten sensors were arrayed in the central line through the jet nozzle along the downwind direction, with the distances of 0.5 m, 1 m, 1.5 m, 2 m, 2.5 m, 3 m, 4 m, 6 m, 8 m, 10 m, to acquire CO2 concentration data.

**Fluent CFD Model Set-up**

The rectangular domain with a cross-section of 6.4 m ×
5.2 m was developed in this work, as shown in Fig. 1. The front of the domain was air inlet, and the rear, named outlet, remained open to the atmosphere. The wind direction was parallel to the bottom from the front to the rear, and a fully developed flow can be established in the computational domain. Structural grid was adopted to discretize the computational domain. Three quantities of cells (i.e., 1133136, 1890864, and 3828672) were utilized to perform the grid sensitivity analysis. SST $k$-$\omega$ model was chosen here. CO$_2$ concentration in the central ground at 200 s after release with the flow speed of 8.8 m s$^{-1}$ was compared, as shown in Fig. 2. It was found that the change in the results was limited and the grid with 1890864 cells was chosen. The minimum horizontal grid size was about 0.0025 m at CO$_2$ inlet. The minimum grid size in the vertical direction was 0.02 m near the ground and expanding away from it with an expansion factor of 1.1 to 0.08 m.

Difference between the wind condition in the experiment and in the simulation can also lead to the deviation between the experimental and simulated cloud concentration (Garcia-Sanchez et al., 2014; Weerasuriya et al., 2018; Zhang et al., 2018). The inlet boundary condition in the CFD simulation was obtained considering the local atmospheric stability class of “F” at the field site. The wind velocity profile was defined by the power law (Tominaga et al., 2008; Wu et al., 2014) to describe the boundary layer.

$$U_Z = U_0 \times \left(\frac{Z}{Z_0}\right)^\alpha$$  \hspace{1cm} (19)

where, the reference velocity $U_0$ and the reference height $Z_0$ were respectively 0.37 m s$^{-1}$ and 2 m, and the value of the power-law exponent $\alpha$ was set as 0.3 according to the literature (Xing et al., 2013). The power law profile was included into the FLUENT code through user-defined functions (UDFs). Air temperature and CO$_2$ temperature were obtained based on experimental data. The initial and boundary conditions are summarized in Table 1.

**Comparison of CO$_2$ Concentration with Various Turbulence Models**

The two cases with CO$_2$ flow speeds of 8.8 m s$^{-1}$ (166.7 L min$^{-1}$) and 13.3 m s$^{-1}$ (250 L min$^{-1}$) were modeled, respectively. The simulation strategy involved a steady-state simulation for flow field and a transient simulation for CO$_2$ cloud dispersion, with the time step of 0.05 s. CO$_2$ concentration data in the central ground line parallel to the wind velocity at 200 s, when the flow field has been relatively steady, were measured. Figs. 3 and 4 show the comparisons between the experimental data and the simulation results using various turbulence models.

The comparisons between experimental data and simulation results show that both of the two turbulence models had a weak accuracy in the near-field region, where the source flow showed strong interaction with wind flow. With the vertical momentum of the source, vortices can be formed in both the upstream and downstream of CO$_2$ inlet, and the flow in the near-field region was dominated by the vortices (Wingstedt et al., 2017). This created highly anisotropic turbulent structure. For the case with CO$_2$ flow speed of 8.8 m s$^{-1}$, stress-$\omega$ model provided the better results in both near- and far-field regions in comparison to SST $k$-$\omega$ model, although SST $k$-$\omega$ model captured the maximum value and the position corresponding to the maximum value. Especially in the near-field region, SST $k$-$\omega$ model significantly underestimated CO$_2$ concentration and the advantage of stress-$\omega$ model was more pronounced.

For the case with CO$_2$ flow speed of 13.3 m s$^{-1}$, the simulation results from stress-$\omega$ model were in good agreement with the experimental data with respect to both the magnitude and trend. It successfully captured the position corresponding to the maximum value and the variation of CO$_2$ concentration in the near-field region that
Fig. 2. Grid independence analysis for flat terrain.

Table 1. The boundary conditions used in the simulation for flat terrain.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Setup</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air inlet</td>
<td>Velocity-inlet</td>
</tr>
<tr>
<td>CO₂ inlet</td>
<td>Velocity-inlet</td>
</tr>
<tr>
<td>Ground</td>
<td>Wall, roughness = 5 × 10⁻³ m</td>
</tr>
<tr>
<td>Top, left, right</td>
<td>Symmetry</td>
</tr>
<tr>
<td>Outlet</td>
<td>Outflow</td>
</tr>
<tr>
<td>Air temperature</td>
<td>293 K</td>
</tr>
<tr>
<td>CO₂ temperature</td>
<td>277 K</td>
</tr>
</tbody>
</table>

decreased firstly then increased with distance. Whereas, the results predicted by SST $k$-$\omega$ model exhibited different law that CO₂ concentration increased with distance. Also, the position of maximum point appeared a certain degree of deviation.

As shown in Table 2, all five performance measures for stress-$\omega$ model were within acceptable range. While, some measures for SST $k$-$\omega$ model were outside, as highlighted in gray. And the main reason is that the strong interaction between wind flow and source flow creates highly anisotropic turbulent structure in the near-field region, and SST $k$-$\omega$ model lacks the capacity to predict accurately the complex flow structure, causing the larger deviation between simulation result and experimental data. The results of the validation metrics support that stress-$\omega$ model can produce much better results compared with SST $k$-$\omega$ model in flat terrain. Therefore, the enhancement of accuracy of simulation results can be considered to be worth the increased computational time.

EVALUATION OF STRESS-$\omega$ MODEL IN URBAN TERRAIN

Description of Wind Tunnel Experiment Considered

In this work, urban terrain was referred to as the street canyon, which was the basic element of urban fabric. In the street canyon, cloud concentration field was mainly governed by the wind field induced by the geometric effects, consisting of wakes, stagnating zones, recirculation, and preferential paths (Park et al., 2015; Mei et al., 2016; Tominaga and Stathopoulos, 2016; Nosek et al., 2017). The experiment (Tan et al., 2018) focused on CO₂ cloud dispersion in the street canyon was simulated for the evaluation of stress-$\omega$ model in cloud dispersion in urban terrain. This experiment was carried out in a 0.75-m-wide, 0.5-m-high wind tunnel. Spires and roughness elements were installed in front of the building arrays to develop the boundary layer. The wind direction was perpendicular to the target street canyon. The incident velocity was measured in the wind tunnel with anemometer at the middle line upstream of the test section to calculate mean velocity and turbulence intensity profile. The reference mean velocity at the building height was 0.66 m s⁻¹ and the exponent $\alpha$ in the power law profile was 0.308. The street canyons were modeled using box-shaped blocks and the CO₂ inlet was a
Table 2. Summary of the statistical performance for flat terrain.

<table>
<thead>
<tr>
<th>Flow rate (m s(^{-1}))</th>
<th>Model</th>
<th>FB</th>
<th>MG</th>
<th>NMSE</th>
<th>VG</th>
<th>FAC2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Perfect model</td>
<td>0</td>
<td>1.0</td>
<td>0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>Acceptable range</td>
<td>-0.3 to 0.3</td>
<td>0.7–1.3</td>
<td>&lt;4.0</td>
<td>&lt;1.6</td>
<td>&gt;0.5</td>
<td></td>
</tr>
<tr>
<td>8.8</td>
<td>SST (k-\omega)</td>
<td>0.166</td>
<td>1.618</td>
<td>0.252</td>
<td>2.282</td>
<td>0.8</td>
</tr>
<tr>
<td></td>
<td>Stress-(k-\omega)</td>
<td>-0.024</td>
<td>0.946</td>
<td>0.0939</td>
<td>1.077</td>
<td>1.0</td>
</tr>
<tr>
<td>13.3</td>
<td>SST (k-\omega)</td>
<td>0.739</td>
<td>3.107</td>
<td>1.505</td>
<td>9.475</td>
<td>0.4</td>
</tr>
<tr>
<td></td>
<td>Stress-(k-\omega)</td>
<td>0.015</td>
<td>0.942</td>
<td>0.147</td>
<td>1.173</td>
<td>0.9</td>
</tr>
</tbody>
</table>

circle with a radius of 0.0065 m located in the target canyon. CO\(_2\) of 99.9\% by volume was jetted vertically upwards at ground level with the flow rate of 4.48 L min\(^{-1}\) under atmospheric pressure, corresponding to the flow speed of 0.5628 m s\(^{-1}\). These two box-shaped blocks used in the experiment had dimensions of 0.2 × 0.05 × 0.05 m\(^3\) (L × W × H) and 0.05 × 0.05 × 0.05 m\(^3\) (L × W × H) respectively, forming five streets connected through a streamwise street. Four sensors based on Infra-Red and detector technology were respectively located near the CO\(_2\) inlet, on the leeward side, on the windward side and above the windward building to acquire CO\(_2\) concentration data. Considering CO\(_2\) inlet as the origin with \(y\) measured as positive in the downwind direction and \(z\) positive upwards, the four measuring points’ coordinates were respectively Point 1 (0, –0.025, 0.025), Point 2 (0.125, –0.025, 0.025), Point 3 (0.125, 0.025, 0.025), and Point 4 (0, 0.05, 0.05).

Fluent CFD Model Set-up

The size of the domain was determined following the wind-tunnel geometry, with width 0.75 m, and height 0.5 m, as shown in Fig. 5. A fully structured grid was built. SST \(k-\omega\) model was also chosen to perform grid-sensitivity analysis among three types of grids, with the number of 1380774, 3183462 and 6135432. Fig. 6 shows the influence of grid size on CO\(_2\) concentration in the centerline of the street at \(z = 0.025\) m and at 15 s after release. The grid with 3,183,462 cells was selected keeping in view both the computing time and the solution accuracy. The grid size in the canyon was 0.005 m and expanding away from it to 0.01 m. Further refinement close to walls and ground was performed.

The inlet boundary conditions used in the simulation were based on the measured incident vertical profiles of mean wind velocity and turbulence intensity in the wind tunnel experiment. The vertical profiles of mean wind velocity, turbulent kinetic energy and its specific dissipation rate were used to describe the variation of wind as a function of height.

\[
\frac{\bar{v}(z)}{\bar{v}(z_H)} = \left(\frac{z}{z_H}\right)^{0.308}
\]

(20)

where \(\bar{v}(z)\) was the mean velocity at \(z\).

\[
k(z) = 1.5 \cdot \bar{v}^2 \left(\frac{z}{z_H}\right) \cdot I^2 \left(\frac{z}{z_H}\right) \left(\frac{z_H}{z}\right)^{0.566}
\]

(21)

where \(I\) was the turbulence intensity.
Fig. 6. Grid independence analysis for urban terrain.

\[
\omega(z) = \frac{2.236 \cdot \nabla(z_H) \cdot I(z_H) \cdot \left( \frac{z_H}{z} \right)^{0.595}}{L_H}
\]

(22)

where \( L \) was turbulence integral scale.

According to the experiment, CO2 was released at an average speed of 0.5628 m s\(^{-1}\). The initial and boundary conditions used in the simulation are shown in Table 3.

**Comparison of CO2 Concentration with Various Turbulence Models**

The time step was \( 1 \times 10^{-3} \) s in the transient simulation to assure Courant number was less than 1. The calculation was carried out up to \( t = 15 \) s, by which time CO2 concentration data at the measuring points were calculated. As shown in Fig. 7, CO2 concentration in urban terrain was larger than in flat terrain due to the blocking effect of spreading downstream. Simulation results reproduced by stress-\( \omega \) model agreed worse with experimental data at all the four measuring points. It underestimated CO2 concentration near the CO2 inlet and on the windward side, and overestimated the concentration on the leeward side and above the windward building. However, SST \( k-\omega \) model underestimated the concentration above the windward building, overestimated the concentration on both the leeward side and windward building, and had the closest coincidence with experimental data near the CO2 inlet.

As shown in Table 4, the simulation results from the two turbulence models were all within acceptable range. And the results also reveal that the performance of stress-\( \omega \) model was worse than that of SST \( k-\omega \) model. This may be due to two reasons. The first is that stress-\( \omega \) model requires more empirical data which can vary from one flow to another, and the advantage itself for complex turbulent flow in urban terrain may be not significant. The second is that an advanced near-wall treatment may play a more important role than the consideration of turbulence anisotropy. In other words, the advantage of SST \( k-\omega \) that automatically switches between the low- and high-Re number \( \omega \) formulation is more significant for the prediction accuracy of flow structure in urban terrain. Coupled with the extra computational effort for the higher number of differential equations, stress-\( \omega \) model still needs further investigation and optimization for accounting for various effects of complex turbulent flow in urban terrain.

**CONCLUSIONS**

This paper performs a comparison of CO2 concentration data obtained by SST \( k-\omega \) model (as the benchmark) and stress-\( \omega \) model with the available wind tunnel test data, to evaluate the applicability and accuracy of RSM for simulating cloud dispersion in flat terrain and urban terrain. The results reflect that stress-\( \omega \) model shows better agreement with experimental data compared to SST \( k-\omega \) model in flat terrain. And it performs better in the far field than in the near-field region. The performance measures for stress-\( \omega \) model are all within acceptable range, while some measures for SST \( k-\omega \) model are outside. For urban terrain, the performance of stress-\( \omega \) turbulence model is worse than that of SST \( k-\omega \) model, although the simulation results are still within acceptable range. This leads to the conclusion that the capacity of RSM is concerned with its application scenario. Specially, stress-\( \omega \) model exhibits
better performance for simulation of the relatively simple flow field in flat terrain and SST k-ω model is still ascendant for the complicated flow structure in urban terrain. The conclusions are of primary importance when deciding which turbulence model to use and drafting guidelines on the use of CFD for the simulation of pollutant dispersion in flat and urban terrains.

It is recommended that the comparison of two-equation model and RSM be made in different terrain conditions. Also, additional experimental data examining the flow structure are necessary to provide a quantitative explanation for the limitation of turbulence models.

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NOMENCLATURE

\begin{itemize}
\item $k$ Turbulent kinetic energy
\item $t$ Time
\item $\varepsilon$ Turbulent dissipation rate
\item $\omega$ Specific turbulent dissipation rate
\item $\delta$ Boundary layer thickness
\item $\nu$ Turbulence dynamic viscosity
\item $\nu_t$ Turbulence kinematic viscosity
\item $\rho$ Density
\item $\tau_r$ Reynolds stress tensor
\item $S$ The strain rate magnitude
\item $P_k$ The production limiter to prevent turbulence buildup in stagnation regions
\item $U$ Velocity vector
\item $i, j$ Grid node in $x$ and $y$ direction
\item $\Omega_{ij}$ The mean-strain-rate tensor
\item $S_{ij}$ The rotation-tensor
\end{itemize}

REFERENCES


