NUMERICAL SIMULATION OF PLUME DISPERSION AROUND AN ISOLATED CUBIC BUILDING: COMPARISON BETWEEN RANS AND LES COMPUTATIONS

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Abstract. The purposes of this study are to confirm the accuracy of LES in modeling plume dispersion near and around a simple building model and to clarify the mechanism of the discrepancy in relation to the RANS computation. Simple LES modeling gives better results than RNG modeling of the distribution of concentration, although the difference for mean velocity is not so large. The horizontal diffusion of concentration is well reproduced by LES. This tendency is closely related to the reproduction of unsteady periodic fluctuation around the cube in LES.

1 INTRODUCTION

Prediction of plume dispersion near buildings is very important for the design of exhaust stacks and air intakes to avoid adverse air quality impacts. Several studies have been carried out on CFD prediction based on a RANS (Reynolds Averaged Navier-Stokes equations) model for dispersion around buildings, but the prediction accuracy is not clear. The authors have examined the performance of various revised k-ε models for the dispersion field around a building and confirmed that all RANS computations under-predicted the horizontal concentration diffusion, although some revised k-ε models yielded much more accurate results than the standard k-ε model [1]. More recently, it was also reported that the underestimation of momentum diffusion observed in conventional RANS computations is mainly because the periodic velocity fluctuation due to vortex shedding around the building is not reproduced [2]. On the other hand, several studies have argued that the results of LES (Large Eddy Simulation) showed good agreement with the experiment in terms of the distributions of mean velocity and turbulence energy around the building, even when the simple sub-grid scale model was used [2, 3]. However, few studies have evaluated the basic performance of LES in modeling the dispersion field for a simple configuration in comparison with the RANS model. The previous studies on LES applied to dispersion around a building...
focused mainly on distributions of concentration in the wake region behind a building [4, 5], and not on those on the building surface, which is closely related to the design of exhaust stacks and air intakes. Especially when an exhaust gas contains toxic, flammable or odorous components, LES, which can evaluate a peak value for concentration, has great advantage compared with RANS.

The purposes of this study are to confirm the accuracy of LES in modeling dispersion near and around a simple building model and to clarify the mechanism of the discrepancy in relation to the RANS computation.

2 COMPUTATIONAL DETAILS

2.1 Flow field

The flow field selected as a test case was that around a cubic building with a flush stack at the rooftop placed within the neutral surface boundary layer (cf. Fig. 1). Wind tunnel measurements were performed by Li and Meroney [6]. The case of a central roof stack with 0° wind direction is adopted in this study. The Reynolds number based on \(H_b\) and \(<u_b>\) was \(1.1 \times 10^4\) (\(H_b\) is the cube height and \(<u_b>\) is the mean inlet velocity at \(H_b\)).

2.2 Numerical method

1) RANS

The RNG k-\(\varepsilon\) model (hereafter RNG), which shows best agreement with the experiment of the four types of turbulence models in the previous study [1], was used. The turbulent Schmidt number was set to 0.7 – see Ref. [8]. The QUICK scheme was used for discretizing momentum and concentration equations. Unsteady calculations were carried out, but results obtained by RNG showed almost no vortex shedding.

2) LES

The standard Smagorinsky model (Smagorinsky constant \(C_S=0.12\)) was used for the sub-grid scale eddy viscosity model [2]. The subgrid scale Schmidt number was set to 0.5 [5]. A second-order centered difference scheme is adopted for the spatial derivatives. For time advancement, the Adams-Bashforth scheme is used for the convection terms and the Crank-Nicolson scheme for the diffusion terms. The computations were conducted for 132 non-dimensional time units \(t^* (=t \times <u_b>/H_b)\) to determine the time averaged values.

2.3 Boundary conditions

The details of the boundary conditions used are provided in Ref. [2]. The computational domain and boundary conditions are summarized in Fig. 1. This domain was discretized into \(86(x_1) \times 76(x_2) \times 46(x_3)\) grids. The minimum grid width was 0.0045\(H_b\). These conditions are the same in both computations. Turbulence in the exhaust outlet velocity was not considered.

1) RANS

The vertical distributions of \(<u_1>\), \(k\) and \(\varepsilon\) at the inflow boundaries were based on the experiment. The generalized log law was used for the solid boundary.

2) LES

A separate LES computation of turbulent boundary layer flow was conducted to generate inflow turbulence. The inflow generating method used here was that proposed by Kataoka and Mizuno [7]. Fig. 2 compares the profiles of mean velocity \(<u_1>\) and turbulence intensity (\(I_{x_1}\)) in streamwise components at the end of a driver section with the experimental values. The
computation accurately reproduced the turbulence property of the inflow condition in the experiment. For the boundary condition at the solid walls, a linear or 1/7 power law distribution of instantaneous velocity was assumed.

Figure 1: Computational domain and boundary conditions (LES).

3 RESULTS AND DISCUSSION

3.1 Velocity distributions

Firstly, the velocity fields without stack emission obtained by RANS and LES computations were determined. The results were compared with the experimental data for the same configuration obtained by the authors, because there were no data of velocity around the cube in reference [6]. In this experiment, wind velocity was measured by a split fiber probe, which can discern three-dimensional components of velocity vector. The Reynolds number based on $H_b$ and $<u_b>$ was $6.4 \times 10^4$.

Table 1 compares the reattachment lengths on the roof ($X_R$) and behind the building ($X_F$). The $X_R$ values obtained by both computations show good agreement with the experimental values, although the value obtained by RNG is slightly larger than the experimental value. On the other hand, $X_F$ is greatly overestimated in RNG as pointed out in the previous study [2], while this discrepancy is much improved in LES.
Fig. 3 shows the profiles of streamwise velocities on the roof and behind the cube at the centerline. The differences between the velocity distributions of the two models were rather small, but the reverse flows on the roof and behind the cube in RNG were a little larger than those in LES as mentioned before. This means that the mixing effect near the cube in LES was stronger than that in RNG.

Fig. 4 compares the velocity vectors on the roof and walls. The reverse flow on the roof in RNG is concentrated more to the centerline than that in LES, that is, larger turbulence mixing occurs in LES.

Table 1: Comparison of reattachment lengths on roof and behind cube

<table>
<thead>
<tr>
<th></th>
<th>X_R</th>
<th>X_F</th>
</tr>
</thead>
<tbody>
<tr>
<td>RNG</td>
<td>0.87H_b</td>
<td>2.46H_b</td>
</tr>
<tr>
<td>LES</td>
<td>0.79H_b</td>
<td>1.54H_b</td>
</tr>
<tr>
<td>Experiment</td>
<td>0.64H_b</td>
<td>1.33H_b</td>
</tr>
</tbody>
</table>

Figure 3: Comparison of vertical distribution of streamwise velocity on roof and behind cube at centerline.

Figure 4: Comparison of velocity vectors on roof and wall surfaces.
3.2 Turbulent energy $k$

The distributions of $k$ on the roof and behind the cube at the centerline are illustrated in Fig. 5. The value of $k$ given by LES is larger than that given by RNG except in the region behind the cube. Peaks of $k$ above the roof are observed in both models, but they are much larger in LES than in RNG. This smaller value of $k$ in RNG is closely related to the stronger reverse flow on the roof in this model than that given by LES.

Fig. 6 shows the distributions of $k$ near the roof and the wall surfaces. The distribution patterns of $k$ in the two models are completely different. A large value of $k$ appears at the edge of the frontal edge of the cube in RNG, while in LES two symmetrical peaks are observed in the upstream region of the roof where the recirculation flow exists (cf. Fig. 4).

![Figure 5: Comparison of vertical distribution of $k$ on roof and behind cube at centerline.](image)

![Figure 6: Contours of turbulent energy $k$ on roof and wall surfaces.](image)

3.3 Mean concentration distributions

Fig. 7 compares the contours of the dimensionless concentration, $K$, on the roof and wall surfaces obtained from the present CFD and the experiment by Li and Meroney [6]. In this study, dimensionless concentration $K$ was defined as $K = \frac{<c>}{<c_0>}$, where $<c_0> = \frac{Q_e}{H_b^2 u_b}$,
<c> is mean concentration and Q_e is the plume flow rate. On the roof surface, the high concentration region (K>100) upwind of the stack in RNG was larger than those in LES and the experiment. The contours of K in RNG also expand greatly in the downstream direction. Generally, RNG underestimates the turbulence diffusion around the cube. This is because the smaller value of turbulent Schmidt number works well in the previous study [1, 8]. On the other hand, the concentrations are widely spread in the horizontal direction in LES. The general distribution of K given by LES is very similar to that of the experiment, although the LES result tends to be a little diffusive. At the side and leeward wall surfaces, the distribution patterns are much different in the two models, and RNG shows smaller value of the concentration than LES. The high concentration region at the side wall in RNG is mainly transferred from the leeward direction by the recirculation flow (cf. Fig. 4(1)), although that in LES is coming from the roof as well as the experiment.

The distribution of K on the centerline of the roof and walls is shown in Fig. 8. Another experimental result with the central vent release for the same configuration by Saathoff et al. [9] was also compared for reference. In the streamwise direction, the values of K given by LES are smaller than those given by RNG. However, in the lateral direction, the LES values are much higher than the RNG values and near the experimental data. In general, the distributions of K obtained by LES show very good agreement. These results are caused by larger lateral turbulence diffusion obtained by LES in comparison with RNG.

![Figure 7: Distribution of time-averaged dimensionless concentration K on roof and wall surfaces.](image)
Fig. 9 indicates the contours of dimensionless concentration $K$ in the near wake region ($x_1/H_b=1.0$). RNG under-predicts the horizontal spread of concentration in comparison with the experiment. However, LES shows better prediction of diffusivity of horizontal concentration, although the vertical diffusion is slightly over-predicted.

Figure 8: Distribution of time-averaged dimensionless concentration $K$ on centerline of roof, leeward and side wall.

Figure 9: Contours of time-averaged dimensionless concentration $K$ in near wake region ($x_1/H_b=1.0$).

### 3.4 Scalar fluxes distribution

Scalar transport of concentration consists of convection and turbulent diffusion effects, which are expressed by the convection as the mean scalar fluxes $<u_i>\langle c \rangle$ and the turbulent diffusion fluxes $<u_i'c'>$, respectively. The convection fluxes can be estimated by using mean velocities and mean concentration. The turbulent diffusion fluxes are calculated directly in LES; on the other hand, in RNG, they are modeled by the gradient diffusion hypothesis,

$$-<u_i'c'> = \nu_t \frac{\partial <c>}{\partial x_i},$$

where $\nu_t$ is eddy viscosity and $Sc_t$ is turbulent Schmidt number.

Fig. 10 compares the streamwise components of the convection flux $<u_1>\langle c \rangle$ and the turbulent diffusion flux $<u_1'c'>$ on the roof. The negative region of $<u_1>\langle c \rangle$ in RNG is much larger than that in LES, because the reverse flow on the roof in RNG is stronger than that in LES, as shown in Fig. 5. On the other hand, the turbulent diffusion flux $<u_1'c'>$ in LES shows a larger value than that in RNG, although the values in both models are rather small in comparison with the convection flux. The LES result shows a large positive peak behind the stack position, which is not observed in RNG.
The lateral components of convection flux \( <u_2'c'> \) and turbulent diffusion flux \( <u_2'c'> \) on the roof are shown in Fig. 11. The peaks of convection flux, \( <u_2>c'> \), which show opposite signs in the two models, are observed on the sides of the stack position. This is because the flow directions in this area are different in the two models (cf. Fig. 4). Furthermore, a large difference between the two models is observed in the distribution of turbulent diffusion flux \( <u_2'c'> \). The result of RNG shows two sharp peaks in the area adjacent to the stack position, which gives opposite signs to the peaks of the convection flux obtained by this model. By contrast, in LES, large values of flux are widely spread in the lateral directions on the roof. These contribute to the diffusive distribution of the mean concentration as shown in Fig. 7(2).

Fig. 12 indicates the contribution ratio of turbulent diffusion fluxes (\( <u_2'c'> \)) to the total scalar transport (\( <u_2>c'>+<u_2'c'> \)) in the lateral direction on the roof. LES shows a much larger contribution of the turbulent diffusion fluxes than RNG. The region with the contribution ratio exceeds 0.8 is spread out from the stack to the side edges of the cube. The good agreement between the mean concentration distributions (cf. Figs. 7 and 8) suggests that the result obtained by LES reproduces the real behavior of concentration transport. It should be noted that the accuracy of turbulent diffusion modeling is very important in predicting the mean concentration distribution.

![Figure 10: Contours of convection flux \( <u_1'>c'> \) and turbulent diffusion flux \( <u_1'c'> \) on roof obtained by LES.](image)
When an exhaust gas contains toxic, flammable or odorous components, its instantaneous as well as its average concentration are of interest. One great advantage of LES is that it can predict fluctuating instantaneous values of concentration.

In this study, the concentration fluctuations are normalized by mean concentration magnitudes to give local and absolute intensities by following Li and Meroney [10]. The local intensity $I_c \left( = \frac{\sqrt{<c^2>}}{<c>} \right)$ is defined as the ratio of the r.m.s. value of the fluctuating concentration to the mean concentration at the same point. The absolute intensity $I_{c_{abs}} \left( = \frac{\sqrt{<c^2>}}{<c_n>} \right)$ is the r.m.s. value of the fluctuating concentration normalized in the same way as the dimensionless concentration, $K$.

Fig. 13(1) shows the concentration distributions of local fluctuation intensity $I_c$ on the roof and the wall surfaces obtained by the present LES computation. At the edge of the cube, very
large values of $I_c$ are observed in comparison with those in the center area of the roof. This means that concentration fluctuation is very large compared with the mean concentration at the frontal edge of the cube. That is, a high concentration peak occurred rarely in this area, and the mean concentration was small. On the other hand, the absolute fluctuation intensity $I_{c_{abs}}$ indicates a different distribution from $I_c$ as shown in Fig. 13(2). The distribution of $I_{c_{abs}}$ is rather similar to that of the mean concentration (Fig. 7), although the region with large values are more spread around the stack position. These properties of the concentration fluctuation are caused by the instantaneous behavior of concentration due to flapping motion of the plume.

Fig. 14 shows the time series of instantaneous fluctuating concentration on the roof. These figures are very different from the time-averaged contours (Fig. 7). The shapes of the high concentration region vary widely in each time step. It should be noted that $t^*$ is defined in section 2.2. These time series show that the plume dispersion around the building is highly unsteady.

(1) Local fluctuation intensity $I_c$  (2) Absolute fluctuation intensity $I_{c_{abs}}$

Figure 13: Concentration fluctuation intensity $I_c$ on roof and wall surfaces obtained by LES.


Figure 14: Time series of instantaneous dimensionless concentration $K$ on roof obtained by LES.

4 CONCLUSIONS

1) Simple LES modeling gives better results than RNG modeling of the distribution of concentration, although the difference between LES and RNG results for mean velocity is not so large. The horizontal diffusion of concentration is well reproduced by LES, due mainly to the reproduction of unsteady periodic concentration fluctuations around the cube.

2) RNG (conventional RANS computation) underestimates the turbulence diffusion near the cube.

3) LES shows a much larger contribution of turbulent diffusion fluxes than RNG. The modeling accuracy of turbulent diffusion is very important for predicting the concentration distribution.

4) LES computation can provide important information on instantaneous fluctuations of concentration, which cannot be obtained by RANS computations.

5) While it is difficult to compare directly the computational time since numerical method and convergence criteria are different between the two methods, the CPU time required to obtain the statistical values in LES is about 25 times more than that in RNG case in the present study.

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