

Large-eddy simulation of reactive pollutant dispersion in a street canyon using a subgrid scale variance model of concentration field

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ABSTRACT: Bi-molecular reactions can affect the transport of air pollutants in urban street canyons. In numerical simulations, we need to evaluate the correlation between the concentrations of the reactants to know the reaction rate. In this paper, we examine the effects of the subgrid scale (SGS) on the reaction rate in large-eddy simulations (LESs). LESs coupled with an SGS variance model are used to study the dispersion of both inert and reactive pollutants in a simulated street canyon. First, we conduct simulations of an inert pollutant at different grid resolutions. The results of these simulations demonstrate the validity of our model for calculating the variance of concentration at the SGS. Second, we apply the model to the dispersion of reactive pollutants. The correlations of the SGS variances become relatively large in a free shear layer at the height of the canyon. However, the SGS variance is very small and has a negligible impact on the mean concentrations of pollutants within the canyon.

KEYWORDS:

Pollutant dispersion; Street canyon; Chemical reaction; LES; Subgrid-scale variance

1 INTRODUCTION

To address an increasing number of air quality issues, many previous studies have evaluated pollutant flow and dispersion in urban areas. Street canyons are a common component of urban areas, and numerous studies have used CFD (computational fluid dynamics) simulations to explore the fundamental characteristics of air pollutant dispersion in street canyons. Additionally, recent increases in computing power have allowed for the development of numerical simulations with high computational loads. In response, engineers and scientists have started to employ large-eddy simulations (LESs) to study the urban atmospheric environment.

Some attempts have been made to extend CFD simulations to the transport of reactive pollutants. For example, Baker et al. [1] and our group [2] have applied LESs with reaction rate models to the dispersion of reactive pollutants in urban street canyons. In these studies, the variance of pollutant concentrations was not considered at the subgrid scale (SGS), which means that the authors assumed perfect mixing of pollutants at the SGS. However, additional studies have reported the influence of the segregation of pollutants at the SGS on the reaction rate [3].

This study aims to assess the influence that the variance of the concentrations at the SGS has on the dispersion of reactive pollutants in an urban street canyon. To evaluate this system, an LES model was coupled with an SGS variance model. To confirm the performance of our model, we initially studied the dispersion of an inert pollutant in an urban street canyon. We then ap-

plied the model to the dispersion of a pollutant that undergoes a bi-molecular reaction in the canyon.

2 MODEL DESCRIPTION AND NUMERICAL METHOD

2.1 LES model of the flow field

We employed a one-equation model for LES proposed by Yoshizawa and Horituti [4]. The model simultaneously solves the transport equation for the kinetic energy at the SGS k_{SGS} and the filtered velocities u_i ($i=1,2,3$). The equations of the model become

$$\frac{\partial \bar{u}_i}{\partial x_i} = 0, \quad (1)$$

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial \bar{u}_i \bar{u}_j}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left(-\tau_{ij} + \frac{2}{Re} \bar{D}_{ij} \right), \quad (2)$$

$$\tau_{ij} - \frac{1}{3} \delta_{ij} \tau_{kk} = -2\nu_{SGS} \bar{D}_{ij}, \quad (3)$$

$$\nu_{SGS} = C_1 \Delta k_{SGS}^{1/2}, \quad (4)$$

$$\frac{\partial k_{SGS}}{\partial t} + \frac{\partial \bar{u}_j k_{SGS}}{\partial x_j} = 2\nu_{SGS} \bar{D}_{ij}^2 - C_2 \frac{k_{SGS}^{3/2}}{\Delta} + \frac{\partial}{\partial x_j} \left[\left(\frac{1}{Re} + C_3 \Delta k_{SGS}^{1/2} \right) \frac{\partial k_{SGS}}{\partial x_j} \right]. \quad (5)$$

In these equations, τ_{ij} is the Reynolds stress at the SGS; D_{ij} is the strain-rate tensor; Re is the Reynolds number; ν_{SGS} is the eddy viscosity coefficient at the SGS; Δ is the grid width; and C_1 , C_2 and C_3 are the model coefficients.

2.2 SGS variance model

The filtered mass conservation of pollutants becomes

$$\frac{\partial \bar{c}_m}{\partial t} + \frac{\partial \bar{u}_j \bar{c}_m}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\left(\frac{1}{ReSc} + \frac{\nu_{SGS}}{\sigma_{tc}} \right) \frac{\partial \bar{c}_m}{\partial x_j} \right] + \bar{R}_m, \quad (6)$$

where Sc is the Schmidt number, σ_{tc} is the turbulent Schmidt number at the SGS, and R_m is the source/sink term due to the reactions.

In this study, we considered the following bi-molecular reaction:



Reaction rates for the reduction of c_1 and c_2 and the corresponding production of c_3 , are defined as

$$\bar{R}_1 = \bar{R}_2 = -\bar{R}_3 = -D_{a1} \overline{c_1 c_2}, \quad (8)$$

where D_{a1} is the first Damköhler number. The filtered product of c_1 and c_2 can be approximated by the following equation:

$$\overline{c_1 c_2} = \bar{c}_1 \bar{c}_2 + \overline{c_1'' c_2''}, \quad (9)$$

where x'' is the SGS variance of x . Following Meeder and Nieuwstadt [3], we employed the transport equation of the SGS correlation described in Equation (10). We numerically integrated it with the governing equations for the flow and the grid scale (GS) concentration fields

$$\frac{\partial \overline{c_1'' c_2''}}{\partial t} + \frac{\partial \overline{u_j c_1'' c_2''}}{\partial x_j} = 2 \frac{\nu_{SGS}}{\sigma_{tc}} \frac{\partial \overline{c_1}}{\partial x_j} \frac{\partial \overline{c_2}}{\partial x_j} + \frac{\partial}{\partial x_j} \left[\left(\frac{1}{ReSc} + \frac{\nu_{SGS}}{\sigma_{tc}} \right) \frac{\partial \overline{c_1'' c_2''}}{\partial x_j} \right] - C_4 \overline{c_1'' c_2''} \frac{k_{SGS}^{1/2}}{\Delta}, \quad (10)$$

where C_4 is a model coefficient.

To validate the performance of the SGS variance model, we carried out a numerical experiment to evaluate the dispersion of a sole scalar without reaction. In this case, $D_{a1} = 0$ and Equation (10) reduces to

$$\frac{\partial \overline{c''^2}}{\partial t} + \frac{\partial \overline{u_j c''^2}}{\partial x_j} = 2 \frac{\nu_{SGS}}{\sigma_c} \left(\frac{\partial \overline{c}}{\partial x_j} \right)^2 + \frac{\partial}{\partial x_j} \left[\left(\frac{1}{ReSc} + \frac{\nu_{SGS}}{\sigma_c} \right) \frac{\partial \overline{c''^2}}{\partial x_j} \right] - C_4 \overline{c''^2} \frac{k_{SGS}^{1/2}}{\Delta}. \quad (11)$$

For this simulation, we set $c_1 = c_2 = c$.

2.3 Computational details

Figure 1 shows an illustration of the street canyon model with an aspect ratio of unity. It has a uniform shape along the y -axis, and the computational domain has a size of $2H(x) \times 2H(y) \times 2H(z)$. A line source of c or c_2 is set at the bottom of the canyon along the center. For the case involving the reactive pollutant, the inflow supplies a constant concentration of c_1 into the domain.

Periodic boundary conditions are applied for all components of the flow fields, both in the stream-wise and span-wise directions. This means that infinitely long street canyons line up continuously along the x -axis. A constant pressure difference is imposed between the inflow and outflow of the computational domain. The upwind wind direction is set to be perpendicular to the street canyon. We carried out the simulation under an isothermal condition.

Calculation conditions are listed in Table 1. The Reynolds number is approximately 1.5×10^5 and is defined with a building height of H and reference velocity of U_{upw} . We set the model constants to be $Sc = 1.0$, $\sigma_{tc} = 0.5$, $C_1 = 0.05$, $C_2 = 1.0$, $C_3 = 0.1$ [4], and $C_4 = 1/Sc$ [5]. Table 2 shows the grid resolutions used in the simulations. We used all of the resolutions for the simulations of the inert pollutant dispersion, whereas only GR32 was employed for the reactive pollutant dispersion. All of the statistics in this paper were averaged along the y -axis because of the uniform shape along the street canyon.

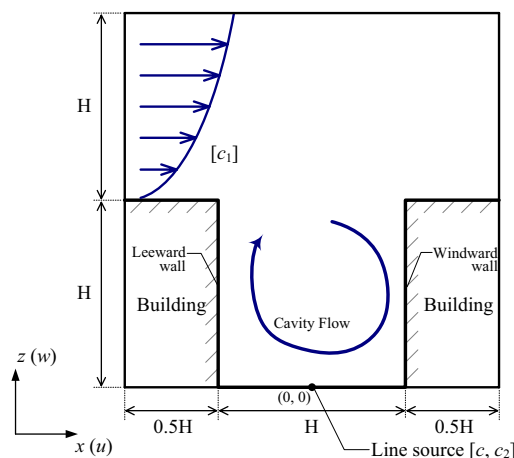


Figure 1. Schematic diagram of the analytical model.

Table 1. Calculation conditions.

Time Marching	PISO (SOR) [6]
Time Discretization	Adams-Bashforth, Crank-Nicolson (Diffusion term in GS NS equation)
Space Discretization	2 nd order Central Difference, FCT scheme (Advection terms in scalar transport equations) [7]
Inflow B.C.	Vel., k_{SGS} : Periodic; Conc.: $c = 0.0$, $c_{1, in} = C_0$, $c_{2, in} = c_{3, in} = 0.0$; Pressure: $p_{in} = p_{out} + 1.2 \times 10^{-2} U_{upw}^{-2}$; SGS conc. variance: Constant (= 0.0)
Outflow B.C.	Vel., k_{SGS} : Periodic; Conc., SGS conc. variance: Gradient-zero
Side B.C.	Periodic
Top B.C.	Vel.: u, v = free-slip, $w = 0$; k_{SGS} , Conc., SGS conc. variance: Gradient-zero
Wall and Ground B.C.	Vel.: linear-1/7 power law; k_{SGS} , Conc., SGS conc. variance: Gradient-zero
Line Source	Conc.: Constant flux (c, c_2)

Table 2. Grid partitionings.

Case	All*	Target canyon**
GR32	64 x 32 x 48	32 x 32
GR64	128 x 64 x 96	64 x 64
GR128	256 x 128 x 192	128 x 128

* $N(x) \times N(y) \times N(z)$; ** $N(x) \times N(z)$ ($z < H$)

3 RESULTS AND DISCUSSION

3.1 Grid resolution and flow field

We initially checked the dependency of the flow field on the grid resolution. Statistics relating to the velocities are normalized by the mean velocity at $z/H = 2.0$ (U_{upw}) in each case.

Figure 2 shows the profiles of the mean stream-wise velocities at three locations. An increase of grid resolution results in high wind-speeds just above the canyon, which makes the cavity eddy stronger in the high resolution case. The difference between the stream-wise velocities for GR128 and GR64 is smaller than the difference between GR64 and GR32. This means that the sensitivity of the flow field to the grid resolution becomes low at a resolution of approximately $H/128$.

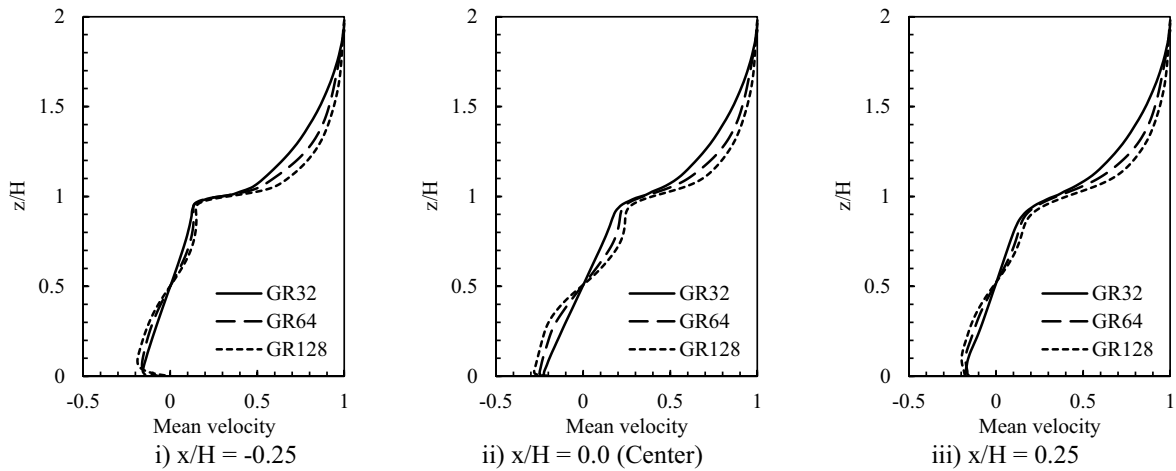


Figure 2. Mean velocity in the stream-wise direction. All variables are normalized by U_{upw} .

The higher resolution enables a larger amount of kinetic energy to be contained in the GS. Therefore, RMS (root-mean-square) values of the filtered velocities become high in GR128 and low in GR32 (Figs 3 i) and ii)). Consequently, the kinetic energy at the SGS (k_{SGS}) is the lowest in GR128 (Fig. 3 iii)).

3.2 Grid resolution and inert scalar field

Before accounting for the reactivity of pollutants, we conducted dispersion simulations for an inert pollutant at the three different grid resolutions. Concentrations presented in this section are normalized by C_n :

$$C_n = Q_e / U_{upw} H L, \quad (12)$$

where Q_e is the emission rate of the pollutant and L is the length of the street canyon.

Figure 4 shows the mean concentration profiles for the inert pollutant. The mean concentration is high along the lower part of leeward wall because it is in the direct downwind region of the line source. Some differences of the mean concentrations are apparent for the different grid resolutions; however, the trend of the dependency on the grid resolution is not clear compared to the flow field in the previous section.

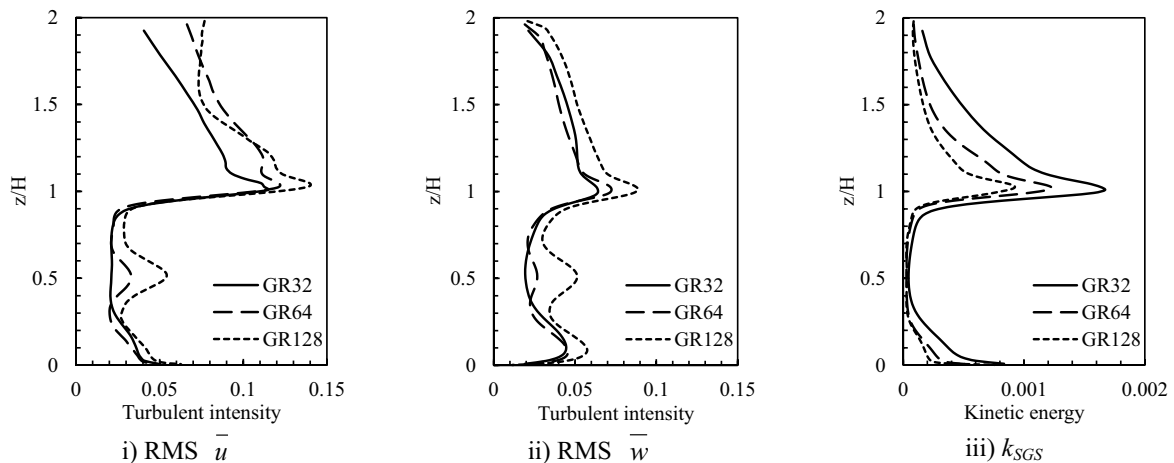


Figure 3. Turbulent intensity at the GS and kinetic energy at the SGS at $x/H = 0.0$ (Center).

All variables are normalized by U_{upw} .

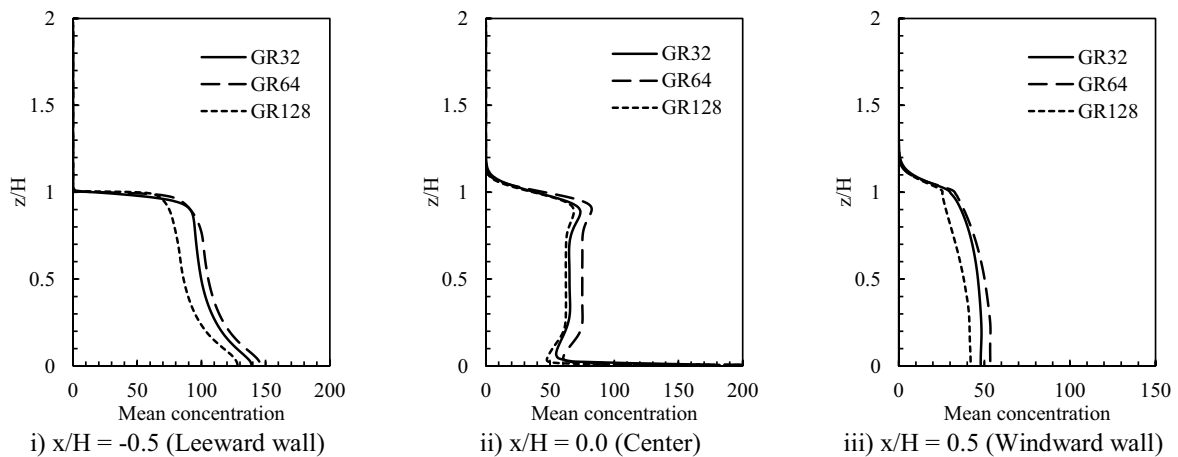


Figure 4. Mean concentration normalized by C_n .

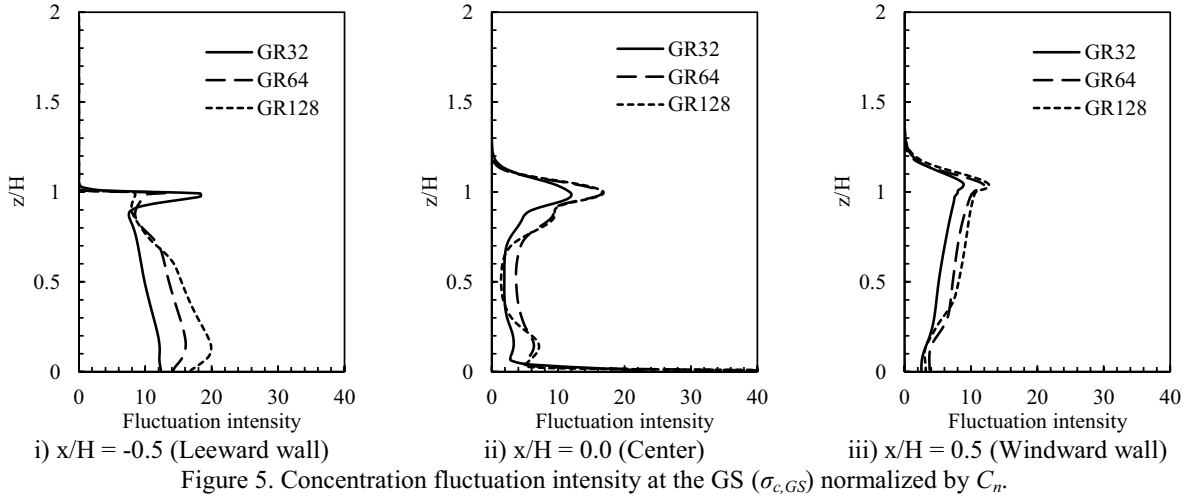


Figure 5. Concentration fluctuation intensity at the GS ($\sigma_{c,GS}$) normalized by C_n .

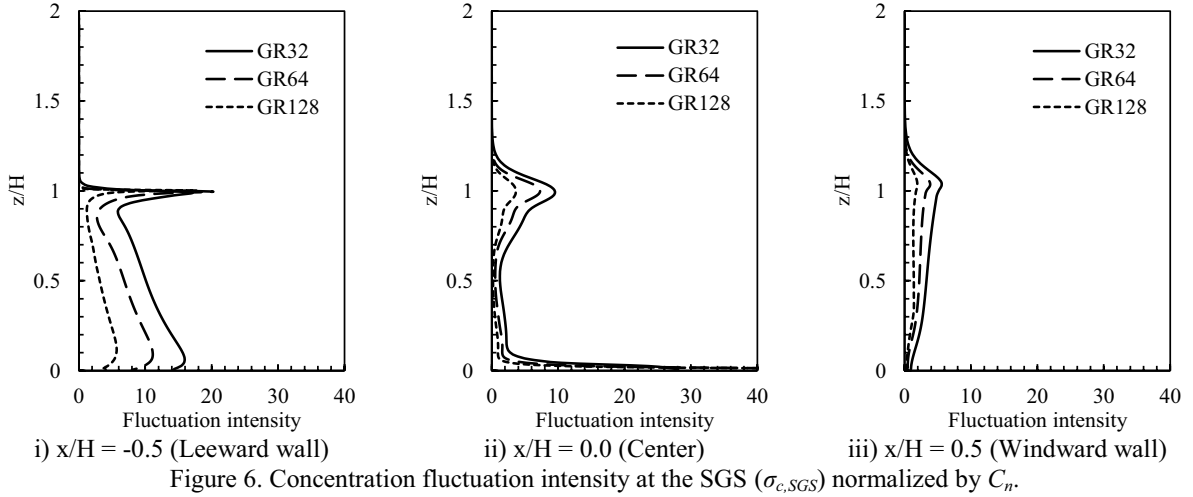


Figure 6. Concentration fluctuation intensity at the SGS ($\sigma_{c,SGS}$) normalized by C_n .

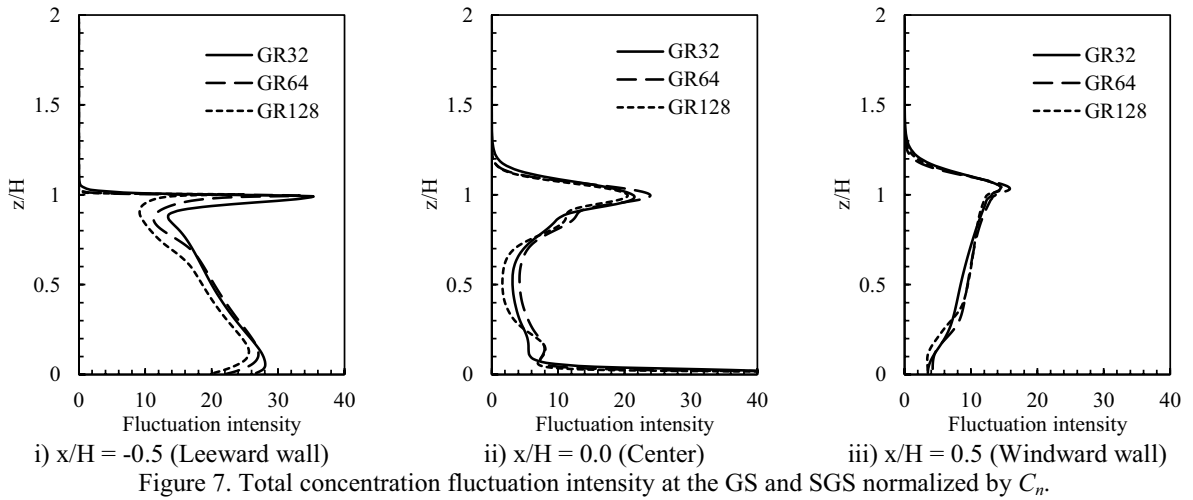


Figure 7. Total concentration fluctuation intensity at the GS and SGS normalized by C_n .

Figures 5 and 6 show the concentration fluctuation intensities at the GS $\sigma_{c,GS}$ and SGS $\sigma_{c,SGS}$, respectively. Here, $\sigma_{c,GS}$ is the RMS of the filtered concentration, and $\sigma_{c,SGS}$ is the mean value of $\overline{c'^2}^{1/2}$. The higher resolution also makes it possible to have more concentration fluctuation energy at the GS. Therefore, $\sigma_{c,GS}$ is highest in GR128 and lowest in GR32, and $\sigma_{c,SGS}$ shows the opposite behavior. Additionally, $\sigma_{c,SGS}$ is greater than $\sigma_{c,GS}$ on the leeward wall for GR32 because the region is near the line source.

We defined the total fluctuation intensity of the concentration σ_c as the sum of $\sigma_{c,GS}$ and $\sigma_{c,SGS}$. Although some discrepancies remain near the top of the leeward wall, Figure 7 shows that σ_c becomes comparable for the three grid resolutions. This means that our SGS variance model worked well to evaluate the variance of the concentration field at the SGS.

3.3 Influence of SGS variance on the dispersion of reactive pollutants

To evaluate the effect of the reaction between c_1 and c_2 , we compared two different cases. The first case accounts for the SGS correlation of c_1 and c_2 to calculate the reaction rates using Equation (10), and the second case neglects it. Concentrations are normalized by C_0 , or the concentration of c_1 in the inflow. D_{a1} has a value of approximately 1.3, and it is defined using U_{upw} , H and C_0 . This value of D_{a1} agrees well with the actual values reported for the reaction between ozone and nitrogen monoxide in urban canyons [2]. The results described in the previous sections demonstrate that sensitivity to the grid resolution remains high for GR32. However, we elected to use this resolution for this portion of the study because we expected that the influence of the SGS variance model would be largest in the case of the lowest resolution.

Figure 8 shows the distributions of the mean concentrations of c_1 and c_2 for the case that includes the SGS variance model. As the reaction proceeds, the concentrations of c_1 and c_2 are reduced in the canyon (Eq. (7)).

The presence or absence of the SGS variance model resulted in small differences between the mean concentrations, as shown in Figure 9. This is because the contribution of the SGS correlation to the reaction rate is very small relative to the product of the filtered concentrations (Eq. (9)). Figure 10 shows that the SGS correlation becomes large at a value of approximately $z/H = 1.0$ due to the strong mixing of c_1 and c_2 . However, the correlation is a small percentage of the product of the filtered concentrations in most regions in the canyon.

4 CONCLUSIONS

To study the dispersion of both inert and reactive pollutants in an urban street canyon, we used LESs that were coupled with an SGS variance model. The model solves the transport equations of the variance or the correlation of pollutants at the SGS with the equations of the filtered concentrations.

First, we validated the performance of the model by evaluating the concentration fluctuations at the SGS for changing grid resolutions. Three resolutions of averaged grid widths ($H/32$, $H/64$ and $H/128$) were employed, where H is the height of the canyon. The concentration fluctuation intensity at the GS was small for the coarse grid case. This was due to the expansion of the filtering width. However, the SGS variance model could estimate the variance lost in the filtering operation. From this result, we concluded that the model could reliably calculate the SGS variance of the concentrations.

Second, we investigated the effect of the SGS variance of concentrations on dispersion for the case of bi-molecular reactions. We carried out simulations at a grid resolution of $H/32$ and either included or excluded the SGS variance model. The correlations of concentration variations at the SGS of reactive pollutants became relatively large at the height of the canyon. This was because

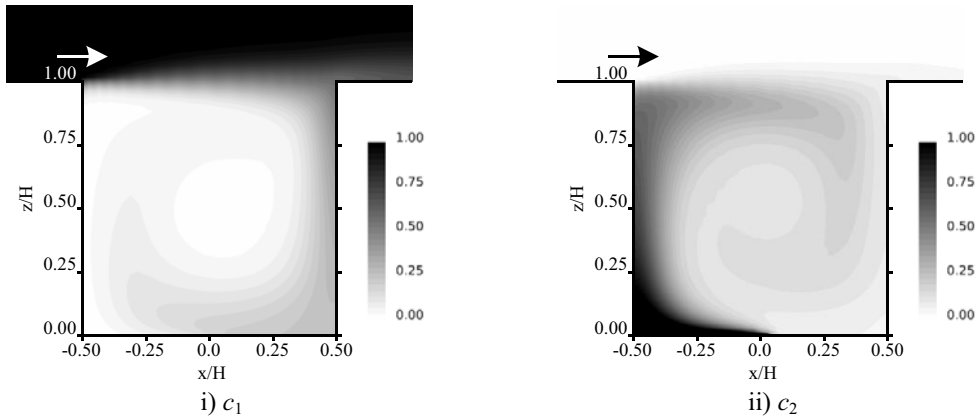
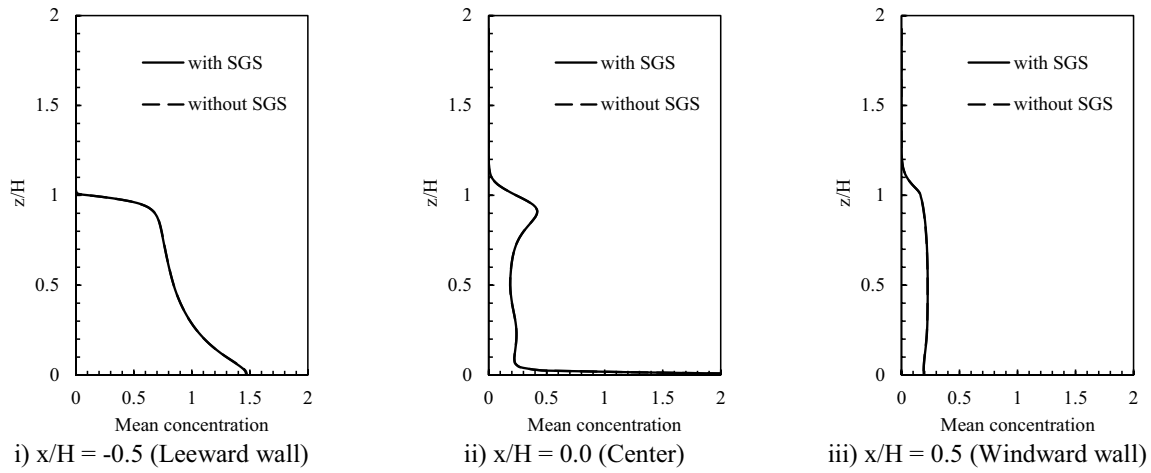
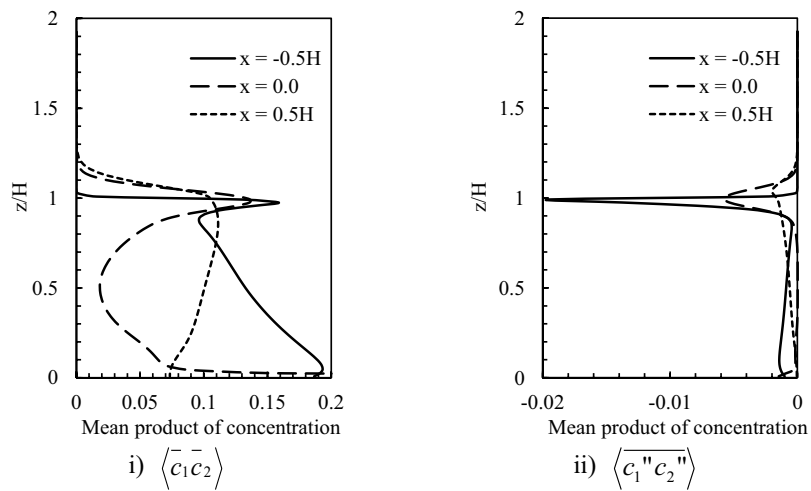


Figure 8. Distributions of the mean concentration of reactive pollutants for the case which accounts for the correlation of c_1 and c_2 at the SGS. These concentrations are normalized by C_0 .



i) $x/H = -0.5$ (Leeward wall) ii) $x/H = 0.0$ (Center) iii) $x/H = 0.5$ (Windward wall)

Figure 9. Comparison of the mean value of c_2 between two cases with and without the SGS variance model. The concentrations are normalized by C_n .



i) $\langle \bar{c}_1 \bar{c}_2 \rangle$ ii) $\langle \bar{c}_1'' \bar{c}_2'' \rangle$

Figure 10. Mean product of the reactive pollutant concentrations in the GS and the SGS normalized by C_0 .

the two pollutants (one came from above the canyon and the other from inside the canyon) were well mixed by the turbulence at this location. However, we found that the SGS variance was too small to make a significant difference in the mean concentrations of pollutants in the canyon.

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CFD modelling of flow and dispersion in the built environment: different RANS models and a first attempt to use URANS

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ABSTRACT: Air pollution is a global phenomenon which has been the subject of study for several years. Pollutants released from rooftop stacks have a tendency to re-enter the same building or an adjacent building in the near vicinity. Complexities in airflow and pollutant transport due to terrain conditions, local topography and buildings make it very difficult to assess plume concentrations. This paper will analyse the role of the unsteady flow and its influence on pollutant dispersion. The effect of a building located upstream to an emitting building which has a roof stack, will be tested in a boundary layer wind tunnel and compared with computational fluid dynamics simulation (CFD). The most used approach for turbulent flow simulation is the Reynolds-averaged Navier-Stokes (RANS) equations. However, it was confirmed that important inaccuracies for dispersion prediction especially in the near-field of an emitting building are usually obtained by RANS. The reason is attributed to the RANS incapability to capture the inherent unsteadiness of flow in the wake of buildings. The influence of different turbulence models was evaluated but no clear improvement to compensate the mentioned inaccuracy was noticed. The effect of unsteady RANS (URANS) was also analyzed in an exploratory way.

KEYWORDS: CFD, Dispersion; Multiple buildings; Pollutants re-ingestion; Schmidt number; Wind tunnel.

1. Introduction

Air pollution is a global phenomenon which has been the subject of study for several years. Complexities in airflow and pollutant transport due to terrain conditions, local topography and buildings make it very difficult to assess plume concentrations (Saathoff et al., 2009). In the built environment increasing exhaust emissions from institutional, industrial buildings and vehicular traffic are inevitable. Toxic and odorous emissions affecting the urban environment and degrading human health are present in every city. One of the most common urban pollution phenomenon is associated with contaminants released from rooftop stacks. Depending on the average airflow, the turbulence of flow and the building-generated turbulence, pollutants can be trapped in recirculation zones and affect sensitive areas as, for example, fresh air intakes. This closed circuit path is known as re-ingestion of pollutants.

In the past, studies performed by Wilson et al., 1998 and Stathopoulos et al., 2008 showed that the presence of a taller upstream building produces higher concentrations on the rooftop of the emitting building. Currently, ASHRAE 2007 gives guidelines for determining plume dilutions for an isolated building without considering the effects of adjacent buildings and local turbulence. Studies performed by Hajra et al., 2010 have shown that ASHRAE 2007 predicts rather unrealistic and overly conservative dilutions. More recently, CFD has been a useful tool in as-