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Large-eddy simulation of reactive pollutant exchange at the top of a street canyon

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ABSTRACT

The exchange of reactive pollutants (NO, NO_2, and O_3) at the top (roof level) of a street canyon are investigated using the parallelized large-eddy simulation model (PALM). The transport equations of NO, NO_2, and O_3 with simple photochemical reactions are combined within the LES model for this study. NO and NO_2 are emitted from an area source located near the canyon floor, and O_3 is included within the ambient air and inflow. A clockwise-rotating vortex appears in the street canyon and transports NO, NO_2, and O_3. NO and NO_2 are transported along the ground and leeward wall and escape from the canyon at the roof level. O_3 enters the canyon at the roof level and is transported along the windward wall. The mean O_3 production rate is generally negative with large magnitudes at and near the roof level and near the windward wall. The chemical reactions reduce the mean NO and O_3 concentrations in the canyon by 31% and 84%, respectively, and increase the mean NO_2 concentration in the canyon by 318%. The exchange of reactive pollutants at the roof level is significantly affected by small-scale eddies at the roof level and low- or high-speed streaks above the canyon. Air in the canyon with high NO and NO_2 concentrations escapes from the canyon when low-speed air parcel appears due to small-scale eddies at the roof level or low-speed streak above the canyon. In contrast, air outside the canyon with a high O_3 concentration enters the canyon when high-speed air parcel appears because of small-scale eddies at the roof level or high-speed streak above the canyon. The time-lagged correlation analysis reveals that NO, NO_2, and O_3 concentrations near the ground are affected by low- or high-speed streaks above the canyon but not significantly affected by small-scale eddies at the roof level.

1. Introduction

With the increasing awareness of urban air pollution and its impacts on health, flow and pollutant dispersion in urban street canyons have been widely investigated in recent decades. Field observations (Rotach, 1995; Allwine et al., 2002; Nelson et al., 2011), wind tunnel experiments (Pavageau and Schatzmann, 1999; Kastner-Klein et al., 2001; Allegrini et al., 2013), and numerical model simulations (Baik and Kim, 2002; Kwak and Baik, 2012, 2014; Kim et al., 2012; Park et al., 2015; Sanchez et al., 2016; Moradpour et al., 2018) have been performed to better understand flow and pollutant dispersion in street canyons. In particular, numerical modeling is a very useful tool for such investigations, because numerical models can provide data with high spatial and temporal resolutions. Comprehensive reviews of numerical modeling of flow and pollutant dispersion in street canyons are given in Li et al. (2006) and Zhong et al. (2016).

Large-eddy simulation (LES) models have been used to study turbulent flow in urban street canyons. Cui et al. (2004) examined turbulent flow in a street canyon using an LES model and found that a large clockwise-rotating vortex appears in a street canyon and flow is more turbulent near the windward wall than near the leeward wall. They also found that flow at the roof level is intermittent and multiscale turbulent events affect flow at the roof level. Letzel et al. (2008) showed that turbulence generated by wind shear dominates at the roof level and makes the circulation in a street canyon intermittent and unstable. Park et al. (2012) examined turbulent flow in a street canyon with heating of the windward wall, canyon floor or leeward wall. Heating of the canyon floor or leeward wall strengthens a large clockwise-rotating vortex in the canyon. In contrast, heating of the windward wall makes the clockwise-rotating vortex small and induces updrafts near the windward wall. Heating of the windward wall, canyon floor or leeward wall increases both turbulent kinetic energy and magnitude of vertical turbulent momentum flux at the roof level.

In addition to turbulent flow, passive pollutant dispersion in urban

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street canyons has been widely studied using LES models. Michioka et al. (2011) examined the process of pollutant removal from a street canyon using an LES model. They found that small vortices at the roof level and low-momentum fluid above the canyon dominate the process of pollutant removal from the street canyon. Chung and Liu (2013) examined the effects of aspect ratio (i.e., the ratio of building height to canyon width) on pollutant removal from street canyons. They found that when the aspect ratio is larger than 0.5, the amount of pollutant escaped from the canyon decreases as the aspect ratio increases. When the aspect ratio is less than 0.5, pollutant escaped from the canyon reenters the canyon and a change in aspect ratio does not affect the amount of escaped pollutant significantly. Liu and Wong (2014) noted that vertical turbulent pollutant flux is larger than vertical mean pollutant flux at the roof level, except near the windward wall. This means that pollutant emitted near the ground is escaped at the roof level by turbulent eddies rather than by mean flow.

The aforementioned LES studies investigated dispersion of passive pollutant. Pollutants emitted in real urban areas are, however, chemically reactive. Considering this point, LES studies of air pollution in street canyons which couple dynamics and chemistry have been performed (Grawe et al., 2007; Zhong et al., 2015). Baker et al. (2004) combined simple photochemical reactions of nitric oxide (NO), nitrogen dioxide (NO_2), and ozone (O_3) within an LES model to examine dispersion of reactive pollutants in a street canyon. They found that NO and NO_2 concentrations are high near the ground and leeward wall and O_3 is entrained into the canyon near the windward wall, resulting in high O_3 concentration near the windward wall. They also found that vigorous O_3 decomposition occurs near the ground and windward wall, while the center of the canyon reaches a chemical equilibrium. Zhong et al. (2017) investigated reactive pollutant dispersion in a deep street canyon using an LES model coupled with complex chemistry of O_3, NO_x (= NO + NO_2), and volatile organic compounds (VOCs). They found that NO_2 and O_3 concentrations in the street canyon in the simulation with the complex chemical reactions are increased by approximately 30–40% compared to those in the simulation with simple chemistry of NO, NO_2, and O_3. They also found that mixing of chemical species is incomplete in the street canyon, i.e., chemical species are segregated from each other. This segregation of chemical species interrupts conversion of NO to NO_2. Kikumoto and Ooka (2012) examined dispersion of reactive pollutants at the roof level using an LES model and found that reactive pollutants escape from the canyon when flow speed becomes slow at the roof level. In contrast, entrance of reactive pollutants from outside the canyon occurs when flow speed becomes fast at the roof level. However, they did not investigate the effects of turbulent structures (e.g., small vortices and low- or high-speed streaks) on reactive pollutant dispersion. Turbulent structures can significantly affect flow speed at the roof level and hence reactive pollutant dispersion. Along with the line of these previous LES studies and as an extension of those studies, it would be interesting to further investigate the relationship between turbulent structures and reactive pollutant exchange at the roof level. This motivates the present study.

In this study, the effects of turbulence on reactive pollutant exchange at the roof level are investigated. Descriptions of an LES model and simulation design are presented in section 2. In section 3, the LES model is validated and simulation results are presented and discussed. In section 4, a summary and conclusions are given.

2. LES model and simulation design

The parallelized LES model (PALM, Maronga et al., 2015) version 4.0 is used in this study. In PALM, the filtered Navier-Stokes equations under the Boussinesq approximation are used. The momentum equation, mass continuity equation, thermodynamic energy equation, and subgrid-scale (SGS) turbulent kinetic energy equation are solved. For the parameterization of SGS turbulent fluxes, the 1.5-order Deardorff (1980) scheme is used. The third-order Runge-Kutta scheme and the fifth-order upwind scheme (Wicker and Skamarock, 2002) are used for time integration and advection terms, respectively.

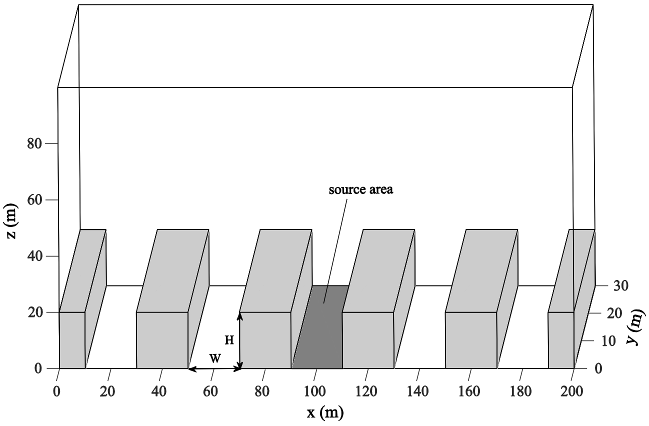

Fig. 1. An illustration of the computational domain. *H* and *W* represent the building height and the width of the street canyon, respectively. NO and NO_2 are emitted in the source area located at the center of the computational domain.

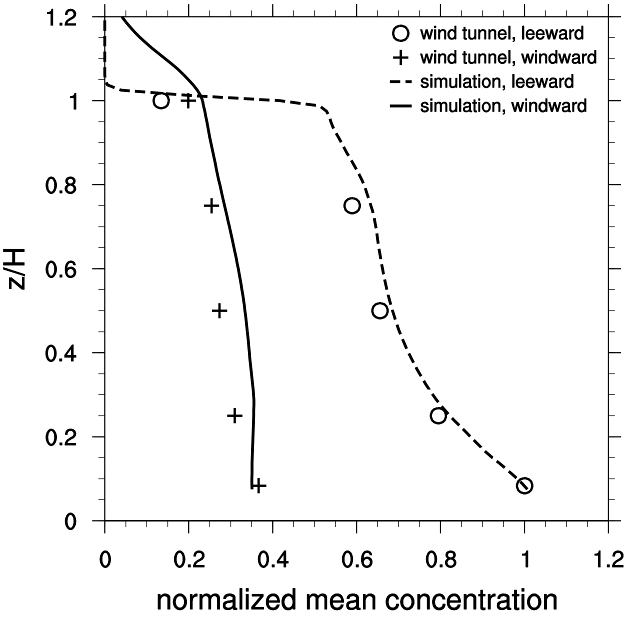

Fig. 2. Vertical profiles of sum of time-averaged NO and NO_2 concentrations (the present simulation result) and passive scalar (the wind tunnel experiment result of Pavageau and Schatzmann (1999)) near the windward and leeward walls (0.03*H* from each wall). The results of the simulation and wind tunnel experiment are normalized by the concentration near the leeward wall at $z = 0.08H$ (Kikumoto and Ooka, 2012). Solid and dashed lines represent the simulation result near the windward and leeward walls, respectively. Cross and open circle represent the wind tunnel experiment result near the windward and leeward walls, respectively.

For this study, the transport equations of NO, NO_2, and O_3 are implemented into PALM. The simple photochemical reactions for NO, NO_2, and O_3 are as follows (Seinfeld and Pandis, 2006):

$$NO_2 + h\nu \rightarrow NO + O, \tag{1}$$

$$O + O_2 + M \rightarrow O_3 + M, \tag{2}$$

$$O_3 + NO \rightarrow NO_2 + O_2. \tag{3}$$

In Eq. (2), M denotes a molecule that absorbs energy and stabilizes O_3, and $h\nu$ denotes a photon of sunlight of frequency ν.

The filtered transport equations of NO, NO_2, and O_3 are expressed