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Modelling the dispersion and transport of reactive pollutants in a deep urban street canyon: Using large-eddy simulation

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ABSTRACT

This study investigates the dispersion and transport of reactive pollutants in a deep urban street canyon with an aspect ratio of 2 under neutral meteorological conditions using large-eddy simulation. The spatial variation of pollutants is significant due to the existence of two unsteady vortices. The deviation of species abundance from chemical equilibrium for the upper vortex is greater than that for the lower vortex. The interplay of dynamics and chemistry is investigated using two metrics: the photostationary state defect, and the inferred ozone production rate. The latter is found to be negative at all locations within the canyon, pointing to a systematic negative offset to ozone production rates inferred by analogous approaches in environments with incomplete mixing of emissions. This study demonstrates an approach to quantify parameters for a simplified two-box model, which could support traffic management and urban planning strategies and personal exposure assessment.

1. Introduction

The term “street canyon” describes a restricted space (poor air ventilation) with surrounding buildings along both sides of the urban street. Vehicle emissions are dominant among various anthropogenic pollutant sources in urbanized areas (Liu et al., 2005). A combination of vehicle emissions and reduced dispersion caused by surrounding buildings could result in poor air quality at the pedestrian level, thereby leading to associated public health effects for those exposed to such environments (Solazzo et al., 2011). Understanding the dispersion and transport of reactive pollutants in urban street canyons is important to effectively quantify – and develop policies to mitigate – such impacts.

Various approaches have been undertaken over recent years to tackle the issue of air pollution inside street canyons. The most fundamental approach is direct field measurement, which can provide first-hand information. Examples of such approach include the studies by Xie et al. (2003), Kumar et al. (2008) and Prajapati et al. (2009). However, there are several disadvantages of field measurements, e.g. challenges to data interpretation, uncontrollable meteorological conditions, low spatial coverage, and high expense. An alternative approach is physical modelling, such as wind tunnels, e.g. Sagrado et al. (2002), Kovar-Panskus et al. (2002), Park et al. (2004) and Michioka et al. (2011), and water channels, e.g. Caton et al. (2003), Jiang et al. (2007) and Li et al. (2008a). Physical modelling offers the advantages of fully controllable test parameters and sampling points so as to provide useful data for the evaluation of numerical models. However, there is a challenge for such models to replicate fully the large-scale atmospheric turbulence of the real world due to scale limitation. Another useful alternative approach is numerical simulation (e.g. computational fluid dynamics, CFD). With rapid development of advanced computer technology, CFD has become a useful tool to explore experimental flow and pollutant dispersion problems (Chang, 2006), providing a complete view of distribution of flow and pollutant fields at high-resolution in both time and space. The most comprehensive applications of CFD have been based on Reynolds-averaged Navier–Stokes (RANS) equations and large-eddy simulation (LES). RANS can only predict mean information about the flow and pollutant fields, while LES also provides the turbulence information about unsteadiness and intermittency (Cai et al., 2008).

The flow patterns in a street canyon under neutral meteorological conditions can be classified into three main regimes (Oke, 1987): isolated roughness, wake interference and skimming flow, depending on the aspect ratio (AR, the ratio of building height H to street width W). Skimming flow, which has been the subject of several studies and will be further investigated here, normally occurs in regular street canyons ($0.7 < AR < 1.5$) and deep street

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canyons (AR > 1.5) (Murena et al., 2009). A single primary vortex is formed within the regular street canyon (e.g. AR = 1), which has been extensively studied. Most studies have only considered passive pollutants (i.e. non-reactive scalars). However, vehicle emissions are chemically reactive, evolving on the time scale of typical canyon circulation and residence times. Such chemical processes are expected to play a role in determining abundance, alongside dispersion and transport, of reactive pollutants. Baker et al. (2004) introduced simple NO_x-O_3 chemistry into a LES model and examined reactive pollutant dispersion and transport inside a regular street canyon (AR = 1). The concept of the photostationary state (PSS) defect was introduced and served as a sensitive indicator of reactive mixing. Baik et al. (2007) carried out a RANS model of a regular street canyon (AR = 1) using the same chemistry as the study by Baker et al. (2004). Both these studies showed that the chemistry is close to equilibrium within the primary canyon vortex, but far from equilibrium at the canyon roof level where air exchange between the canyon and the overlying background takes place. Kikumoto and Ooka (2012) investigated the transport and dispersion of atmospheric pollutants within a regular street canyon (AR = 1) by using LES coupled with a bimolecular chemical reaction ($O_3 + NO \rightarrow$ product). They found that NO_x and O_3 have contrasting mechanisms of transport and the correlation between the reactants' concentration fluctuations strongly influences the reaction rates at the canyon roof level. Kwak and Baik (2012) and Kwak et al. (2013) employed a RANS model coupled with the carbon bond mechanism IV (CBM-IV) considering the chemistry of O_3, NO_x and volatile organic compounds (VOCs) in idealized street canyons (AR = 1, 2). They found that both O_3 and OH oxidation processes are of vital importance in canyon-scale chemistry and that there are two counter-rotating vortices in the street canyon with AR = 2. According to Li et al. (2009), there are multiple vortices within a deep street canyon, which may create very poor ventilation conditions for pollutants. Thus the dispersion of pollutants in a deep street canyon could be substantially different from the AR = 1 case, very complex in terms of both dynamical and chemical processing, and deserves a thorough examination.

This study investigates the dispersion and transport of reactive pollutants in a deep urban street canyon (AR = 2). The LES methodology coupled with a simple chemical mechanism is employed as described in Section 2. In Section 3, the results of the LES dynamical model are evaluated against a water-channel experiment, and the characteristics of reactive pollutant dispersion from the LES coupled with the simple NO_x-O_3 chemistry are presented. An alternative two-box model framework is developed. Finally, the conclusions are presented in Section 4.

2. Methodology

2.1. Numerical model

2.1.1. Flow equations

The LES model employed here is OpenFoam v2.1.1 (OpenFOAM, 2012), in which incompressible flow and neutral conditions are assumed. The filtered momentum equations and continuity equations are

$$\frac{\partial \overline{u}_i}{\partial t} + \frac{\partial}{\partial x_j}\overline{u}_i\overline{u}_j = -\Delta P\delta_{i1} - \frac{\partial \overline{p}}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} + \upsilon\frac{\partial^2 \overline{u}_i}{\partial x_j \partial x_j} \tag{1}$$

$$\frac{\partial \overline{u}_i}{\partial x_i} = 0 \tag{2}$$

where the overbar ($\bar{\bullet}$) represents the filtered quantity, $\overline{u}_i$ (i = 1,2,3) are the filtered velocities, ΔP is the large-scale kinematic pressure difference, δ_{ij} is the Kronecker delta, $\overline{p}$ is the filtered kinematic pressure, υ is the kinematic molecular viscosity and τ_{ij} represents the sub-grid scale (SGS) stresses, which are parameterised as follows:

$$\tau_{ij} = -2\upsilon_{SGS}S_{ij} \tag{3}$$

$$S_{ij} = \frac{1}{2}\left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i}\right) \tag{4}$$

$$\upsilon_{SGS} = C_k k_{SGS}^{1/2}\Delta \tag{5}$$

$$\Delta = (\Delta_1\Delta_2\Delta_3)^{1/3} \tag{6}$$

$$\frac{\partial k_{SGS}}{\partial t} + \frac{\partial}{\partial x_i}(k_{SGS}\overline{u}_i) = 2\upsilon_{SGS}S_{ij}S_{ij} + (\upsilon + \upsilon_{SGS})\frac{\partial^2 k_{SGS}}{\partial x_i \partial x_i} - C_\varepsilon\frac{k_{SGS}^{3/2}}{\Delta} \tag{7}$$

where k_{SGS} is the SGS turbulent kinetic energy, Δ_i (i = 1,2,3) are the local grid spacings and the modelling constants $C_k = 0.094$, $C_\varepsilon = 1.048$.

This study simulates the high Reynolds number (~10^6) turbulent flow (see Section 2.2) in a deep street canyon with rough surfaces and the logarithmic law of the rough-wall (Schlichting and Gersten, 2000) is applied for the near-wall treatment:

$$\overline{u}_{||} = \frac{u_\tau}{\kappa}\ln\frac{z_\perp}{z_0} \tag{8}$$

where $\overline{u}_{||}$ is the resolved scale velocity component parallel to the wall, u_τ is the wall friction velocity, κ (=0.42) is the von Kármán constant, $z_\perp$ is the distance normal to the wall and z_0 (=0.015 m representing a characteristic physical length of 0.15 m, e.g. window frames) is the aerodynamic surface roughness length. u_τ is calculated by Equation (8) and used to derive υ_{SGS} near the wall using

$$\upsilon_{SGS} = \frac{u_\tau^2}{\left|\nabla\overline{u}_{||}\cdot\hat{n}\right|} - \upsilon \tag{9}$$

where $\hat{n}$ is the unit vector normal to the wall.

2.1.2. Equations for reactive pollutants

The reactive pollutants concerned here are nitric oxide (NO), nitrogen dioxide (NO_2) and ozone (O_3). The associated chemical reactions are (Carpenter et al., 1998):

$$NO_2 + h\nu \rightarrow NO + O \tag{10}$$

$$O + O_2 + M \rightarrow O_3 + M \tag{11}$$

$$O_3 + NO \rightarrow NO_2 + O_2 \tag{12}$$

where M denotes a third-body molecule (usually O_2 or N_2) which absorbs excess energy so that O and O_2 may recombine to form an O_3 molecule. The filtered equations for the concentrations of reactive pollutants are: