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# Large-eddy simulation of flow and scalar dispersion in rural-to-urban transition regions



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#### ABSTRACT

Large-eddy simulations (LES) are performed to simulate the flow and scalar transport in rural-to-urban transition regions. The LES framework is first validated with wind-tunnel experimental data of scalar dispersion within and above a staggered array of cubes. It is then used to simulate the scalar dispersion in transition regions from a flat homogeneous terrain to uniform arrays of cubes with height *h*. Staggered cube arrays with five different plan area densities, equal to 0.028, 0.063, 0.111, 0.174 and 0.250, and two incoming wind directions ( $\alpha$ ), equal to 0° and 27° are considered. Above the cube array, self-similar profiles for the mean scalar concentration are found and a scalar internal boundary layer is identified in all the cases. For all the cases tested, larger internal boundary layer thickness is found for  $\alpha = 27^{\circ}$ . Compared with that of  $\alpha = 0^{\circ}$ , which is related to the higher effective surface roughness in the cases of  $\alpha = 27^{\circ}$ . Within the urban canopies, the scalar concentration is found to adjust quickly within the cube array, which leads to a similar scalar concentration distribution pattern after the second row of cubes. Comparing the cases of the two different  $\alpha$ , similar scalar concentration and adjustment pattern are found when the density is low. However, when the density is higher, higher scalar concentration is found in the cases of  $\alpha = 27^{\circ}$  compared with those of  $\alpha = 0^{\circ}$ .

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#### 1. Introduction

The dispersion of scalars within and above urban canopies is a complex process that is affected by various factors such as scalar source location, wind direction, building configuration, turbulence and thermal stability. It has been widely investigated using different methods like field measurements (Davidson et al., 1995; Macdonald et al., 1997; Yee and Biltoft, 2004), wind tunnel experiments (Barlow and Belcher, 2002; Davidson et al., 1996; Gailis and Hill, 2006; Macdonald et al., 1998; Pascheke et al., 2008) and numerical simulations (Boppana et al., 2014; Branford et al., 2011; Cai et al., 2008; Inagaki et al., 2012; Liu and Wong, 2014).

Many studies have focused on the scalar dispersion from point sources. Davidson et al. (1996) performed wind tunnel experiments of plume dispersion through aligned and staggered arrays of obstacles with a scalar point source in front of the arrays. They found that, even within urban canopies, the spanwise profiles of the plumes have a Gaussian shape and are self-similar. For the vertical profiles, self-similarity is not observed in general and a reflected Gaussian plume model can be used to fit the results. In addition, the urban canopy is found to cause a significant increase

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http://dx.doi.org/10.1016/j.ijheatfluidflow.2016.04.004 S0142-727X(16)30119-9/© 2016 Elsevier Inc. All rights reserved. in the vertical height of the plume. Similarly, Macdonald et al. (1997; 1998) performed field and wind tunnel experiments to study the dispersion of a scalar through regular arrays of cubes. They again found that, at a distance beyond two rows of obstacles downstream of the scalar source, the concentration profiles can be well approximated by a Gaussian distribution laterally and a reflected Gaussian vertically. They demonstrated that the plume width increases by a factor of 2-4 with an increase in obstacles width-to-height aspect ratio from one to infinity (two-dimensional canyon). Gailis and Hill (2006) also performed wind tunnel experiments that reproduced the conditions of the field experiments of Yee and Biltoft (2004) to study the scalar dispersion within an obstacle array and then fitted the Gaussian and reflected Gaussian models to the lateral and vertical concentration profiles, respectively. They commented that the development of a physicsbased functional form of mean concentration profiles, instead of being only empirically fitted with a Gaussian model, is necessary. Recently, large-eddy simulation (Philips et al., 2013) and direct numerical simulation (Branford et al., 2011; Coceal et al., 2014) studies were conducted to investigate scalar dispersion from point sources at different locations within urban canopies. They focused on the passive scalar dispersion above a square array of cubes with a plan area density  $\lambda_p = 0.25$  and found that the lateral dispersion is enhanced in the oblique wind case. The plan area density is defined as the total plan area of the obstacles divided by the total surface area. Meanwhile, enhanced ventilation and dispersion are found when the source is put at a street intersection instead of at the middle of a street. Philips et al. (2013) also studied the scalar dispersion from a point source in a staggered array of buildings of various heights with  $\lambda_p = 0.25$ , and investigated the growth of the plume width and height with distance.

To model the dispersion of heat, air pollutants (due to vehicular emissions) or humidity in cities, the scalar source is in fact more suitable to be considered as an area source instead of a point source. The majority of studies that focused on area scalar sources have considered the scalar dispersion in two-dimensional (2D) street canyons. Barlow and Belcher (2002) developed the naphthalene sublimation technique in their wind tunnel experiments to model the scalar dispersion from ground-level area sources within and above 2D street canyons. The area sources modeled in this way correspond to sources with constant scalar concentration. The scalar transfer coefficients for street canyons of different street widths were then studied and the maximum value at an aspect ratio of about 0.7 was identified. For 2D street canyons, different large-eddy simulation studies focused on the turbulent transport of passive scalar concentration (Cheng and Liu, 2011a; Liu and Barth, 2002; Liu and Wong, 2014; Wong and Liu, 2013) and heat (Cai, 2012; Cheng and Liu, 2011b; Li et al., 2012; 2010) within and above the street canyons. These LES studies in general confirmed the importance of turbulent transport for the ventilation and pollutant removal from 2D street canyons especially with high building-height to street-width aspect ratios. Unstable stratification increases the mean wind and turbulence within street canyons and this in turn enhances the ventilation and pollutant removal. For arrays of obstacles, Pascheke et al. (2008) further used the naphthalene sublimation technique to simulate the scalar dispersion (from a confined area source) above arrays of obstacles with uniform and non-uniform heights. Using the data of Pascheke et al. (2008), Boppana et al. (2010) validated their LES model and investigated the different scalar dispersion patterns in arrays of obstacles of uniform and non-uniform heights. By performing large-eddy simulations, Inagaki et al. (2012) investigated the coherent flow structure and Castillo et al. (2011) investigated the characteristics of the urban boundary layer above a square array of cubes with  $\lambda_p$  = 0.25. Boppana et al. (2014) studied the effects of thermal stratification of the flow on the drag and heat transfer of an array of staggered cubes of  $\lambda_p = 0.25$ .

For all the studies mentioned above about the scalar dispersion in three-dimensional urban building arrays with an area scalar source, the focus is on large uniform cube arrays with well developed flows above. However, in real cities, rural-to-urban surface transitions are very common. They can be located near the edges of cities and also in the centre of cities such as parks, lakes, or open areas surrounded by groups of buildings. In this study, the effects of rural-to-urban surface transitions on the scalar dispersion from streets are investigated. In Section 2, the LES framework is introduced. In Section 3, the framework is validated with the wind-tunnel experimental data of Pascheke et al. (2008). In Section 4, the LES results of flow and scalar dispersion in different rural-to-urban transition regions are presented and discussed. Finally, in Section 5, the main results are summarized and conclusions are drawn.

#### 2. LES framework

The LES code solves the filtered continuity equation, the filtered incompressible Navier–Stokes equations in rotational form (Orszag and Pao, 1975) and the filtered scalar transport equation:

$$\frac{\partial \tilde{u}_i}{\partial x_i} = 0,\tag{1}$$

$$\frac{\partial \tilde{u}_i}{\partial t} + \tilde{u}_j \left( \frac{\partial \tilde{u}_i}{\partial x_j} - \frac{\partial \tilde{u}_j}{\partial x_i} \right) = -\frac{\partial \tilde{p}^*}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} + \nu \frac{\partial^2 \tilde{u}_i}{\partial x_j^2} + f_i + F_i, \quad (2)$$

$$\frac{\partial \tilde{\theta}}{\partial t} + \tilde{u}_i \frac{\partial \tilde{\theta}}{\partial x_i} = -\frac{\partial q_i}{\partial x_i} + \frac{\nu}{\mathsf{Sc}} \frac{\partial^2 \tilde{\theta}}{\partial x_i^2} + f_\theta + F_\theta, \tag{3}$$

where  $\tilde{u}_i$  is the filtered velocity in the *i* direction (with i = 1, 2, 2) 3 corresponding to the streamwise (x), spanwise (y) and vertical (z) direction, respectively),  $\tilde{\theta}$  is the filtered scalar concentration,  $\tilde{p}^* = \tilde{p}/\rho + \frac{1}{2}\tilde{u}_i\tilde{u}_i$  is the modified kinematic pressure,  $\tilde{p}$  is the filtered pressure,  $\rho$  is the density of air,  $\nu$  is the kinematic viscosity, Sc is the Schmidt number for molecular diffusion of  $\theta$  in air,  $\tau_{ij} = u_i \tilde{u}_j - \tilde{u}_i \tilde{u}_j$  and  $q_i = u_i \tilde{\theta} - \tilde{u}_i \tilde{\theta}$  are the subgrid-scale (SGS) stress tensor and scalar fluxes, respectively. The terms  $f_i$  and  $f_{\theta}$ are the immersed forcing terms used to simulate the effects of the blocks on the flow and scalar concentration, respectively. The term  $F_i$  is a mean pressure gradient forcing term, and  $F_{\theta}$  is a source term of the scalar. Neutrally-stratified conditions are considered and therefore no additional term is required to account for the effect of buoyancy. The modulated gradient SGS model (Lu and Porté-Agel, 2010; 2013) was used here to calculate  $\tau_{ii}$  and  $q_i$ . It computes the structure of the  $au_{ij}(q_i)$  based on the normalized gradient vector, which is derived from the Taylor expansion of the exact  $\tau_{ii}$  ( $q_i$ ). The local equilibrium hypothesis is used to evaluate the SGS kinetic energy and the SGS scalar concentration scale. The SGS flux magnitude is then computed as the product of the SGS velocity scale (which is proportional to the square root of the SGS kinetic energy) and the SGS scalar concentration scale. The main advantages of the model include: (i) the model satisfies material frame indifference, (ii) it is simple and computationally inexpensive as neither test filtering nor additional transport equation is needed, and (iii) it is able to capture flow anisotropy better than eddy-viscosity models.

In all the simulations, the top boundary was considered as a stress-free wall with zero vertical scalar flux. For the bottom wall, the boundary condition was based on the Monin–Obukhov similarity theory (Businger et al., 1971). Although the theory is only valid for averaged quantities under steady and homogeneous conditions, it is commonly used also to fluctuating (LES filtered) quantities in both homogeneous and heterogeneous flows. Even though recent studies have highlighted the limitations of this approach (e.g., Abkar and Porté-Agel, 2012; Chamorro and Porté-Agel, 2010; Marusic et al., 2001), no alternative is available for complex flows. Under neutral conditions, the surface shear stress  $\tau_{13, 5}(x, y, t)$  (i = 1, 2) is often computed as (Stoll and Porté-Agel, 2006; 2008)

$$\tau_{i3,s}(x, y, t) = -\left[\frac{\kappa \tilde{u}_r(x, y, z, t)}{\ln(z/z_0)}\right]^2 \frac{\tilde{u}_i(x, y, z, t)}{\tilde{u}_r(x, y, z, t)},$$
(4)

where the subscript *s* denotes surface values, *t* is the time,  $\tilde{u}_r(x, y, z, t) = [\tilde{u}_1(x, y, z, t)^2 + \tilde{u}_2(x, y, z, t)^2]^{1/2}$  is the local instantaneous (filtered) horizontal velocity magnitude at height  $z = \Delta_z/2$ , and  $z_0$  is the aerodynamic surface roughness length. Similarly, if a scalar area source with a fixed concentration at the surface was used, the surface scalar flux  $q_{3,s}(x, y, t)$  was computed as:

$$q_{3,s}(x, y, t) = -\frac{\kappa^2 \tilde{u}_r(x, y, z, t) [\theta(x, y, z, t) - \theta_s(x, y, t)]}{\ln(z/z_0) \ln(z/z_{0\theta})},$$
(5)

where  $\theta_s$  is the scalar concentration at the surface and  $z_{0\theta}$  is the aerodynamic surface roughness length for scalar. Here,  $z_{0\theta} = z_0$  is assumed. The spatial derivatives in the horizontal directions were calculated based on the pseudo-spectral method, while a second-order central-difference method was used in the vertical direction. The time advancement was carried out using the second-order Adams–Bashforth scheme (Canuto et al., 1988). More details on the LES code can be found in Albertson and Parlange (1999), Porté-Agel et al. (2000), Porté-Agel (2004), Stoll and Porté-Agel (2006),

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