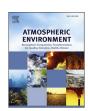
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Stochastic backscatter modelling for the prediction of pollutant removal from an urban street canyon: A large-eddy simulation



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HIGHLIGHTS

- A comparison of scalar removal from a street canyon using 2 LES SGS models is made.
- The SGS model with stochastic backscatter increases the exchange velocity by ~15%.
- This is shown to be in better agreement with a wind-tunnel dataset.
- Consequently, mean canyon concentration is ~15% lower with the backscatter model.

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ABSTRACT

The large-eddy simulation (LES) approach has recently exhibited its appealing capability of capturing turbulent processes inside street canyons and the urban boundary layer aloft, and its potential for deriving the bulk parameters adopted in low-cost operational urban dispersion models. However, the thin roof-level shear layer may be under-resolved in most LES set-ups and thus sophisticated subgridscale (SGS) parameterisations may be required. In this paper, we consider the important case of pollutant removal from an urban street canyon of unit aspect ratio (i.e. building height equal to street width) with the external flow perpendicular to the street. We show that by employing a stochastic SGS model that explicitly accounts for backscatter (energy transfer from unresolved to resolved scales), the pollutant removal process is better simulated compared with the use of a simpler (fully dissipative) but widely-used SGS model. The backscatter induces additional mixing within the shear layer which acts to increase the rate of pollutant removal from the street canyon, giving better agreement with a recent wind-tunnel experiment. The exchange velocity, an important parameter in many operational models that determines the mass transfer between the urban canopy and the external flow, is predicted to be around 15% larger with the backscatter SGS model; consequently, the steady-state mean pollutant concentration within the street canyon is around 15% lower. A database of exchange velocities for various other urban configurations could be generated and used as improved input for operational street canyon models.

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1. Introduction

With over half of the world's population living in urban areas (WHO, 2015), it is important to understand the effects of the densely built environment on the transportation and dispersion of pollutants emitted near ground-level. Street canyons form a key constituent part of the urban fabric (Oke, 1988), and particular concern surrounds the case of vehicular emissions released within

* Corresponding author. E-mail address: x.cai@bham.ac.uk (X.-M. Cai). deep street canyons (i.e. $H/W \gtrsim 0.7$, where H is the building height and W is the street width), in which a 'skimming flow' regime is established (Oke, 1987). In this regime, the bulk of the flow passes over the street canyon, leaving pollutants largely trapped within the canyon and thus susceptible to build up to potentially harmful levels. An extreme case occurs when the oncoming wind is exactly perpendicular to the street axis, which has been observed to lead to particularly poor ventilation, and thus poor air quality (DePaul and Sheih, 1985; Xie et al., 2003).

The associated risks to human health have led to an extensive number of controllable (idealised) experiments being attempted in order to better understand wind flow and dispersion characteristics for the perpendicular skimming flow regime. These experiments include reduced-scale wind-tunnel (Meroney et al., 1996; Kastner-Klein and Plate, 1999; Pavageau and Schatzmann, 1999; Brown et al., 2000; Simoëns and Wallace, 2008; Salizzoni et al., 2009; Blackman et al., 2015) and water-channel (Baik et al., 2000; Li et al., 2008; Di Bernardino et al., 2015) testing, as well as numerical computational fluid dynamic (CFD) modelling (Baik and Kim. 1999. 2002: Liu and Barth, 2002: Walton and Cheng, 2002: Cui et al., 2004; Li et al., 2005; Liu et al., 2005; Cai et al., 2008; Cheng and Liu, 2011; Michioka et al., 2011; Cai, 2012; Liu and Wong, 2014). CFD models offer a number of advantages over laboratory experiments, including lower set-up and running costs, significantly better spatial coverage, and the ability to test a variety of urban configurations with relative ease. They typically fall into one of two categories: Reynolds-averaged Navier-Stokes (RANS) models, which parameterise all turbulence length-scales in search of the mean flow and dispersion patterns; and large-eddy simulation (LES) models, which parameterise only the smallest turbulence length-scales (whilst resolving the larger scales) and retrieve the mean spatial patterns by time-averaging the instantaneous model output record (Vardoulakis et al., 2003; Li et al., 2006). LES is computationally more expensive than RANS but offers greater simulation accuracy. For example, Walton and Cheng (2002) compared the performance of RANS and LES for simulating pollutant dispersion in a street canyon of unity aspect ratio (i.e. H/W = 1) and found the LES-predicted mean concentration patterns to be in much better agreement with wind-tunnel data. This was due to the model's ability to capture important unsteadiness in the canyon's primary recirculating vortex, which was observed to lead to puffs of pollution being intermittently ejected from the canyon rather than being steadily dispersed away, as simulated by RANS. The dominating influence of intermittent events on tracer release from a street canyon was also observed in the wind-tunnel experiment of Simoëns and Wallace (2008), who concluded that a simple mean concentration gradient model applied to the Reynolds-averaged transport equation would be insufficient to model scalar fluxes. The importance of capturing unsteadiness in simulations of dispersion around buildings has also been demonstrated in other LES-RANS comparison studies, e.g. Dejoan et al. (2010), Tominaga and Stathopoulos (2010), Salim et al. (2011a, 2011b). LES is thus better suited to derive input parameters for simpler operational street canyon models, which is recently being attempted (e.g., the DIPLOS project – http://www.diplos.org).

To achieve adequate simulation accuracy with LES, the choice subgrid-scale (SGS) model, which parameterises the effects of the unresolved scales of motion on the resolved ones, is often critical (Mason, 1994). This is particularly true in under-resolved flow regions where the small-scale motions carry an appreciable fraction of the turbulent energy. For street canyon flow, Letzel et al. (2008) showed that Kelvin Helmholtz waves generated within the rooflevel shear layer significantly affect the behaviour of a dispersing tracer. However, with substantially fine resolution (at least 100 across-canyon grid points) required to explicitly resolve these waves, much of the shear layer dynamics is often unavoidably handled by the SGS model. This poses a significant challenge to even the most complex SGS models available. O'Neill et al. (2016) argued that backscatter (transitory transfer of turbulent kinetic energy from unresolved to resolved scales by eddy interactions that produce larger wavelengths) is an important process within the roof-level shear layer that should therefore be explicitly considered in the SGS model. Use of the popular Smagorinsky (1963) SGS model, which only parameterises forward energy transfer (i.e. it is fully dissipative), has been found to under-predict the primary vortex strength inside the street canyon (Cui et al., 2004). With the dynamic SGS model (Germano et al., 1991; Lilly, 1992), which only

accounts for partial backscatter through locally reduced eddy-viscosities (strong backscatter requires negative values, which are typically prohibited), similar deficiencies can also be observed (Cheng and Liu, 2011; Liu and Wong, 2014). Alternatively, O'Neill et al. (2016) employed an SGS model that explicitly accounts for backscatter using a stochastic forcing term in the momentum equation (Mason and Thomson, 1992). This increased the momentum transfer across the shear layer, thus driving an intensification of the primary vortex, bringing it significantly closer towards wind-tunnel observations (Brown et al., 2000).

The next step, and the aim of the present paper, is to test what effect the backscatter model has on the prediction of pollutant removal from the street canyon. To achieve this, we compare LES output from two separate simulations of scalar transport in a street canyon of unit aspect ratio; one adopting the Smagorinsky SGS model, and the other adopting the stochastic backscatter SGS model. The paper is structured as follows. Section 2 provides a mathematical overview of the LES methodology, as well as the two different SGS models adopted in this study (the Smagorinsky model and the stochastic backscatter model). Section 3 describes the LES model configuration settings for each simulation. We then present the results and discuss the implications in Section 4. Finally, conclusions are drawn in Section 5.

2. Mathematical formulation

2.1. LES overview

LES numerically solves the filtered Navier—Stokes and continuity equations on a discretised grid. The filter separates the larger eddies, which are resolved by the model, from the smaller eddies, which are not resolved and must therefore be parameterised. For an incompressible fluid, the governing equations (using tensor notation) are given by:

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j},\tag{1}$$

$$\frac{\partial u_i}{\partial x_i} = 0, \tag{2}$$

where u_i is the filtered (resolved) velocity component in the direction x_i , p is the filtered pressure, t is time, ρ is the (constant) air density, τ_{ij} is the turbulent SGS stress tensor, and where viscous effects have been assumed to be negligible compared with the turbulent SGS stresses for the large Reynolds number flow. The term involving τ_{ij} represents the effects of the unresolved velocity field on the resolved field, and is handled by the SGS model.

In addition, the filtered transport equation can be solved to represent the dispersion of a passive scalar:

$$\frac{\partial C}{\partial t} + u_j \frac{\partial C}{\partial x_i} = -\frac{\partial \sigma_i}{\partial x_i} + S, \tag{3}$$

where *C* is the filtered scalar field, *S* is a source term, and σ_j are the SGS scalar fluxes, which again must be handled by the SGS model.

2.2. Smagorinsky SGS model

The net effect of the unresolved turbulent stresses is to drain energy from the resolved flow (forward energy transfer) to the SGS field. The Smagorinsky SGS model is a purely dissipative model that seeks to parameterise this net energy transfer using a subgrid-scale eddy-viscosity, $v_{\rm SGS}$, in an analogous way to molecular diffusion:

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