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Technical note

Source depletion analogy for reactive plume dispersion over schematic urban areas

Zhangquan Wu, Chun-Ho Liu*

Department of Mechanical Engineering, The University of Hong Kong, Hong Kong

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ABSTRACT

Gaussian plume models have been used to estimate pollutant distribution for decades. In view of the empirically determined dispersion coefficients (largely based on atmospheric stability), their application in urban setting needs to be interpreted cautiously. It is even more complicated if chemically reactive pollutants are considered. In this technical note, we examine the reactive plume dispersion over schematic urban areas in attempt to excel the functionality of the conventional Gaussian plume models. Open-channel flows over an array of identical ribs in crossflows serve the theoretical platforms of atmospheric surface layer (ASL) over buildings. The irreversible ozone O_3 titration oxidizes nitric oxide to nitrogen dioxide NO_2, representing the typical anthropogenic air pollution chemistry. Large-eddy simulation (LES) is employed to calculate the flows and pollution physics/chemistry coupling around/over the explicitly resolved roughness elements. The LES results show that, unlike the (larger) mesoscale ones, the conventional approach of modifying dispersion coefficients in terms of the timescales of pollution physics/chemistry is inapplicable due to inhomogeneous vertical mixing. We thus switch to the source depletion analogy which, however, estimates well the concentrations only above the plume rise mean height. A noticeable discrepancy is caused by the dominated oxidation in the near-wall region. Finally, the regression of LES output shows that the vertical dimensionless concentrations exhibit the Gamma γ-distribution for a range of background O_3 concentrations, unveiling a new, primitive parameterization of reactive plume dispersion over urban areas.

1. Introduction

Air pollution poses major threat to premature mortality (Lelieveld et al., 2015) but its levels over 80% of the cities in the world are unhealthy (WHO, 2016). Most air pollutants are chemically reactive that evolve to their secondary counterparts in the atmospheric boundary layer (ABL). The conventional Gaussian plume model (Roberts, 1923) has been widely employed in practical problems (Moreira et al., 2006), regulatory enactment (Briant et al., 2013), air toxic assessment (Scheffe et al., 2016) as well as continental pollutant transport (Tsuang et al., 2003). Its results, however, must be interpreted cautiously because of the inert-pollutant assumption (Harrison and McCartney, 1980) and the complicated near-wall turbulent transport processes in the atmospheric surface layer (ASL; Britter and Hanna, 2003).

In view of dense buildings, dispersion schemes have been developed to handle the rapid mixing in urban ASLs (Briggs, 1973). The widening plume coverage is attributed to the elevated turbulence kinetic energy (TKE) in response to ground-level aerodynamic resistance (Walcek, 2002). Early Gaussian plume models adopted the power-law wind profile (Sharma and Myrup, 1975) together with the empirically determined dispersion coefficients (Skupniewicz and Schacher, 1986) to handle the enhanced pollutant transport over urban areas. Whereas, the solution approach was basically site specific (Venkatram et al., 2005) that hindered from the understanding of fundamental mechanism. Extensive field measurements (Mavroidis and Griffiths, 2001), laboratory experiments (Chung et al., 2015) and mathematical modeling (Inagaki et al., 2012) have been conducted to elucidate the influence of rough surfaces on ASL transport processes. However, the functional form of plume dispersion is not yet developed likely because of complicated urban morphology.

ABL pollutants are seldom mixed uniformly with ambient air in view of the inhomogenity in both flows and sources (Georgopoulos and Seinfeld, 1986). Chemical kinetics and dynamics are therefore coupled with each other to modify the pollutant compositions which, however, are often ignored in reactive plume dispersion models (Chiogna et al., 2010). Mathematical modeling has been adopted for air pollution physics/chemistry coupling, such as the chemical evolution of nitrogen oxides NO_x (= NO + NO_2; where NO and NO_2 are nitric oxide and

* Corresponding author. Department of Mechanical Engineering, 7/F, Haking Wong Building, The University of Hong Kong, Pokfulam Road, Hong Kong.
E-mail address: liuchunho@graduate.hku.hk (C.-H. Liu).

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nitrogen dioxide, respectively), for decades (Lamb and Seinfeld, 1973). In the engineering community, modeling turbulent transport by computational fluid dynamics (CFD) is generally grouped into stochastic (Bullin and Dukler, 1974), deterministic (Wang and Zhang, 2009) and large-eddy simulation (LES; Tseng et al., 2006).

Simple, non-CFD models, such as AERMOD (USEPA, 2016) and CALINE4 (Benson, 1984), possess the benefit of quick solution together with the ability performing multiple simulations concurrently. To the authors' best knowledge, perhaps due to the challenging pollution physics/chemistry coupling in inhomogeneous flows, there is no non-CFD model developed so far for reactive plume dispersion over urban areas. It therefore motivates our interest in rapid, non-CFD modeling techniques for pollutant-concentration estimates. This section introduces the problem background and reviews the existing literature. The theory of reactive plume dispersion is detailed in Section 2. The solution approach, computation configuration and numerical methods are described in Section 3. The findings, especially the turbulent transport processes and the newly proposed non-CFD, reactive plume parameterization (Gamma γ-distribution), are reported in Section 4. Conclusions are finally drawn in Section 5.

2. Theoretical background

The irreversible ozone O_3 titration

$$NO + O_3 \xrightarrow{k_3} NO_2 + O_2 \tag{1}$$

is considered where O_2 is oxygen molecule and k_3 ($= 0.411\ \text{ppm}^{-1}\,\text{s}^{-1}$) the chemical reaction rate constant at 293.15 K. The consumption (production) rates of nitric oxide and ozone (nitrogen dioxide) by chemistry Equation (1) are equal to

$$\frac{d\overline{c}_{NO}}{dt} = \frac{d\overline{c}_{O_3}}{dt} = -\frac{d\overline{c}_{NO_2}}{dt} = -k_3 \times \overline{c}_{NO} \times \overline{c}_{O_3} \tag{2}$$

where c_ϕ is the concentration of chemical species ϕ and overbar $\overline{\psi}$ the resolved-scale component in the LES. Hence, the chemistry timescales of nitric oxide $\tau_{NO} = 1/k_3\overline{c}_{O_3}$ and ozone $\tau_{O_3} = 1/k_3\overline{c}_{NO}$. Given the model configuration of uniform inflows doped with a constant background ozone concentration $[O_3]_0$, our preliminary LES results show that the ozone consumption $\Delta[O_3]$ ($= [O_3]_0 - \langle\overline{c}_{O_3}\rangle$ where angle brackets $\langle\psi\rangle$ denote the ensemble averaged properties) is less than 10%. We therefore essentially assume a constant chemistry timescale of nitric oxide $\tau_{NO} = 1/k_3[O_3]_0$ in the following analyses.

3. Methodology

3.1. Mathematical model

LES of the open-source CFD code Open-FOAM 2.3.0 (OpenFOAM, 2015) is used in this technical note. The flows are assumed to be isothermal and incompressible that are calculated by the continuity and the Navier-Stokes equations in filtered variables. Source terms $\mathscr{S}_\phi$, which handle the chemical kinetics in the irreversible ozone titration Equation (1), are integrated into the filtered convection-diffusion equation

$$\frac{D}{Dt}\phi = \mathscr{D}(\phi) + \mathscr{S}_\phi \tag{3}$$

for the transport of chemical species ϕ where D/Dt is the material derivative and $\mathscr{D}(\phi)$ the diffusion term. Here, the source terms in the transport equations of NO, NO_2 and O_3 are $\mathscr{S}_{NO}$ ($= -k_3\overline{c}_{NO}\overline{c}_{O_3}$), $\mathscr{S}_{NO_2}$ ($= k_3\overline{c}_{NO}\overline{c}_{O_3}$) and $\mathscr{S}_{O_3}$ ($= -k_3\overline{c}_{NO}\overline{c}_{O_3}$), respectively. Hence, the source terms for NO and O_3 are consumptions while NO_2 production. The subgrid-scale (SGS) motions are modeled by the Smagorinsky model (Smagorinsky, 1963). The one-equation SGS model is employed to enforce SGS TKE conservation (Schumann, 1975). Only resolved scales are included in the source terms $\mathscr{S}_\phi$. The timescales are compared by the dimensionless Damköhler number Da ($= \tau_p/\tau_\phi$; where τ_p and τ_ϕ are the timescales of physical and chemical processes, respectively; Janssen et al., 1990). We focus on the mixing processes so the diffusion timescale τ_d is used to measure the physical processes. We look into the reactive plume dispersion of nitric oxide so its chemical timescale τ_{NO} is used to measure the chemical processes.

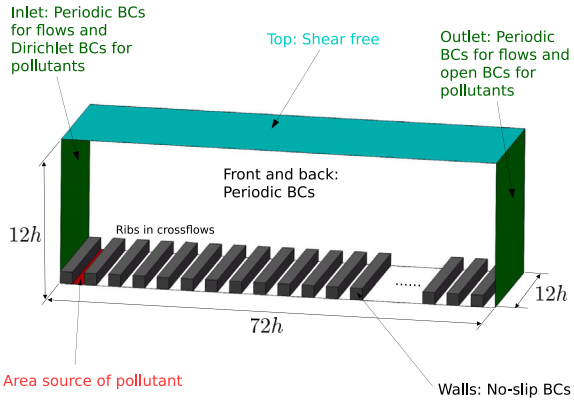

Fig. 1. Spatial domain of the LES.

The LES model for schematic urban area consists of a number of idealized urban street canyons fabricated by identical square ribs of size h (Fig. 1). The spatial domain sizes $72h$ (length) × $12h$ (width) × $12h$ (height) that is composed of 36 idealized street canyons of the same geometry. The street width b is the same as the building height h so the building-height-to-street-width (aspect) ratio is equal to unity. The flows thus fall into the skimming flow regime (Oke, 1988). The prevailing flows in the urban ASL are driven by the (background) pressure gradient perpendicular to the street axes, representing the worst scenario of pollutant removal from street canyons. Ensemble average of the LES-calculated pollutant concentrations $\langle\overline{c}_\phi\rangle$ is applied in the homogeneous spanwise y direction in the data analyses. The infinitely long streamwise x domain for flows is constructed by periodic boundary conditions (BCs). Wall BCs are applied on all the solid boundaries and shear-free BCs ($\partial\overline{u}/\partial z = \partial\overline{v}/\partial z = \overline{w} = 0$) along the domain top $z = H$. The prevailing wind enters the computational domain from the upstream inflow doped with a constant background ozone concentration $[O_3]_0$. The sensitivity to NO chemistry timescales τ_{NO} is tested by controlling $[O_3]_0$ (Table 1). An area source of nitric oxide with constant concentration $[NO]_0$ is placed on the ground surface of the first street canyon that serves as a reactive pollutant being continuously emitted into the computational domain, simulating the vehicular exhaust in urban areas. Neumann BCs of pollutants ($\partial\overline{c}_\phi/\partial z = 0$) are applied on the remaining solid and shear-free boundaries. An open BC of pollutants ($\partial\overline{c}_\phi/\partial t + \overline{u}\,\partial\overline{c}_\phi/\partial x = 0$) is prescribed at the downstream outflow so all the chemical species are removed from the computational domain without reflection. The entire computational domain is discretized into 4.6×10^6 (hexahedral) cells approximately.

Table 1
Root mean square (RMS) error comparing source depletion model and Gamma γ-distribution.

Background ozone concentration $[O_3]_0$ (ppb)	RMS error	
	Source depletion model	Gamma γ-distribution
1	0.009745	0.001761
10	0.0006537	0.002166
50	0.008048	0.002672
100	0.01582	0.002972
200	0.02984	0.003605
500	0.05867	0.004318

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