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Original Article

A numerical investigation of reactive air pollutant dispersion in urban street canyons with tree planting

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ABSTRACT

Vegetation acts as a momentum and thermal sink, affecting the mixing of species and temperature-dependent constants of reaction rates. Numerical simulations were performed to investigate the effects of vegetation on the dispersion of reactive pollutants using a computational fluid dynamic (CFD) model coupled with NO-NO₂-O₃ photochemistry. Moreover, characteristics of temperature and flow fields were analyzed for different aspect ratios and leaf area densities. The results showed that flow is reversed in the presence of trees, and it enhances as leaf area density (*LAD*) increases; additionally, vegetation creates downward and vortex flows. The results also revealed that the dispersion of nitrogen oxides is influenced by the flow patterns; nevertheless, chemical reactions are significant for the dispersion of ozone. In addition, the vegetation is observed to weaken ventilation efficiency of NO and NO₂; however, ventilation efficiency of O₃ improves in *LAD* = 0.5 and 1.0. Aspect ratios and leaf area densities are also found to interact with each other; consequently, the optimum *LAD* is different for each aspect ratio. The larger regions with maximum concentrations of nitrogen oxides at the height of 2 m for aspect ratios of 0.5, 1.0, and 2.0 correspond to *LAD* = 2.0, 1.5, and 1.0, respectively. Furthermore, vegetation as compared to tree-free environment, mostly leads to a better chemical equilibrium.

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1. Introduction

In recent years, air pollution in cities worldwide has turned into a major social problem as it damages human health. Traffic emission in the road network of urban environment is an effective factor on air quality control (Colville et al., 2001). Emissions are dispersed into the atmosphere by advection and diffusion mechanisms. Buildings around emission sources act as barriers, decreasing air pollutant dilution and ventilation. Street canyon aspect ratio is defined as the ratio of building height to the street width (Chang and Meroney, 2003; Oke, 1987; Scungio et al., 2015) and heating/cooling of building facades (Sini et al., 1996; Xie et al., 2005) are among other parameters which alter flow and dispersion. In addition, vegetation acts as a momentum sink and causes flow field to change, thereby

making different patterns of concentrations. The influence of trees on pedestrian air quality is dependent on vegetation design (Janhäll, 2015), and it is larger for larger aspect ratios of street canyons (Buccolieri et al., 2009). Results of simulations done by Salim et al. (2011b) showed that the presence of avenue-like tree planting in an urban street canyon causes the overall concentration level to increase owing to reduction of air recirculation. Amorim et al. (2013) reported that the aerodynamic effect of trees on the dispersion depends on wind direction, and wind direction of nearly parallel to the main avenue can decrease concentrations. Wania et al. (2012) evaluated the effect of vegetation on particle dispersion using the ENVI-met model, and found that increasing both aspect ratio of street canyon and vegetation density causes lower ventilation and higher concentrations of particles. In a recent study by Vranckx et al. (2015) stated that seasonal leaf loss of trees affects the annual average impacts of trees, and trees cause the annual average concentration to increase, which is dependent on vegetation type. Moreover, the cooling intensity of vegetation is significant. For instance, Baik et al. (2012) realized that roof greening improves air quality near roads, since cool air near the roof flows inside the canyon and strengthens ventilation and dilution of pollutants.

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Atmospheric pollutants used in modeling investigations have usually been assumed to be passive or inert; nonetheless, they are chemically reactive. Baker et al. (2004) studied the dispersion of reactive air pollutants using a large eddy simulation (LES) model, which included the photochemistry reactions of NO, NO₂, and O₃. Subsequently, Baik et al. (2007) and Kang et al. (2008) employed a RANS model to investigate the effect of bottom heating in a street canyon on the flow and dispersion of the reactive pollutant. Bai (2010) applied an empirical model to analyze photochemical processes of ozone for several sky conditions and obtained good agreement between measured and calculated concentrations of ozone. Using an LES model coupled with a bimolecular reaction model, Kikumoto and Ooka (2012a) identified that the mixing of reactive gases within a two-dimensional canyon causes the reactions to proceed, and the concentrations of products to increase. Zhong et al. (2015) observed two vertically-aligned vortices within a street canyon with an aspect ratio of 2, and presented a simple two-box model to examine the interplay of dynamics and chemistry. Murena (2012) also employed two-box model and measurement data in order to analyze carbon monoxide dispersion in a deep street canyon with an aspect ratio of 5.8, and obtained good correlation between real and modeled data. Park et al. (2015) used a coupled CFD-chemistry model to investigate characteristics of flow and reactive pollutant dispersion in urban street canyons with different aspect ratios, and studied interaction between aspect ratios and six different emission scenarios. The evaluation of urban trees influence on ozone concentration from Washington, DC, to central Massachusetts using meteorological, emission, and air quality models showed that urban trees locally decrease ozone concentration, but increase overall regional concentration (Nowak et al., 2000). Salmond et al. (2013) measured concentrations of nitrogen oxides at street level and one floor up within a street canyon in Auckland, New Zealand, and observed that during the foliated season, mean concentration increases below tree top due to reduction of upward transport of emissions.

The above literature review reveals that gases in the atmosphere are influenced by the interaction between vegetation and chemical reactions in microscale environments. This study aims to investigate the effects of vegetation on the dispersion of reactive air pollutants in the urban environment using a computational fluid dynamic model coupled with photochemistry of NO_x-O₃. In order to identify effects of vegetation, the tree-free environment is simulated and its results are compared with the results of environments that include different foliage conditions. Furthermore, street canyons with three different aspect ratios are modeled to examine flow and dispersion patterns.

2. Methods

2.1. Numerical model

A three-dimensional computational fluid dynamic model based on the Reynolds-averaged Navier–Stokes equations (RANS) model was used in this study which was closed by the realizable *k*- ϵ turbulence model (Shih et al., 1995) with standard wall functions (Launder and Spalding, 1974) which are modified for roughness as described by Cebeci and Bradshaw (1977). Natural convection mechanism of heat transfer was considered using the incompressible ideal gas law to calculate the density of each chemical species. Besides energy equation, the P1 radiation model was used to simulate solar radiation. Furthermore, the numerical model contained transport equations for Nitric oxide (NO), nitrogen dioxide (NO₂), and ozone (O₃) with the photochemistry reactions, which reacts in the presence of sunlight (Carpenter et al., 1998):



where M stands for a third-body molecule (O₂ or N₂ or another third molecule) which absorbs excess energy so that O reacts with O₂ to produce O₃ molecule. Therefore, the transport equations are:

$$\begin{aligned} \frac{\partial \overline{[\text{NO}]}}{\partial t} + \frac{\partial}{\partial x_i} (\overline{u_i [\text{NO}]}) &= D \frac{\partial^2 \overline{[\text{NO}]}}{\partial x_i \partial x_i} + \frac{\partial}{\partial x_i} \left(K_c \frac{\partial \overline{[\text{NO}]}}{\partial x_i} \right) + J_{\text{NO}_2} \overline{[\text{NO}_2]} \\ &\quad - k_1 \overline{[\text{O}_3]} \overline{[\text{NO}]} + S_{\text{NO}}, \end{aligned} \quad (4)$$

$$\begin{aligned} \frac{\partial \overline{[\text{NO}_2]}}{\partial t} + \frac{\partial}{\partial x_i} (\overline{u_i [\text{NO}_2]}) &= D \frac{\partial^2 \overline{[\text{NO}_2]}}{\partial x_i \partial x_i} + \frac{\partial}{\partial x_i} \left(K_c \frac{\partial \overline{[\text{NO}_2]}}{\partial x_i} \right) \\ &\quad - J_{\text{NO}_2} \overline{[\text{NO}_2]} + k_1 \overline{[\text{O}_3]} \overline{[\text{NO}]} + S_{\text{NO}_2}, \end{aligned} \quad (5)$$

$$\begin{aligned} \frac{\partial \overline{[\text{O}_3]}}{\partial t} + \frac{\partial}{\partial x_i} (\overline{u_i [\text{O}_3]}) &= D \frac{\partial^2 \overline{[\text{O}_3]}}{\partial x_i \partial x_i} + \frac{\partial}{\partial x_i} \left(K_c \frac{\partial \overline{[\text{O}_3]}}{\partial x_i} \right) + k_2 \overline{[\text{O}]} \overline{[\text{O}_2]} \overline{[\text{M}]} \\ &\quad - k_1 \overline{[\text{O}_3]} \overline{[\text{NO}]}, \end{aligned} \quad (6)$$

In Eqs. (4)–(6), *D* is the molecular diffusivity, *K_c* the eddy diffusivity, *J_{NO2}* the photolysis rate of NO₂ for the reaction in (1), *k₁* the rate constant for the reaction in (3), and *k₂* the rate constant for the reaction in (2). *S_{NO}* and *S_{NO2}* represent the source terms of NO and NO₂, respectively. The turbulent Schmidt number *Sc_t* is considered to be 0.5 as determined by Gromke and Blocken (2015a). According to the pseudo-steady-state approximation for the highly reactive chemical species such as oxygen atom (O) in the above reactions, the formation rate of O by Reaction (1) is the same as the depletion rate of O by Reaction (2) (Seinfeld and Pandis, 1998). Hence,

$$k_2 \overline{[\text{O}]} \overline{[\text{O}_2]} \overline{[\text{M}]} = J_{\text{NO}_2} \overline{[\text{NO}_2]}, \quad (7)$$

As a result, Eq. (6) can be rewritten as:

$$\begin{aligned} \frac{\partial \overline{[\text{O}_3]}}{\partial t} + \frac{\partial}{\partial x_i} (\overline{u_i [\text{O}_3]}) &= D \frac{\partial^2 \overline{[\text{O}_3]}}{\partial x_i \partial x_i} + \frac{\partial}{\partial x_i} \left(K_c \frac{\partial \overline{[\text{O}_3]}}{\partial x_i} \right) + J_{\text{NO}_2} \overline{[\text{NO}_2]} \\ &\quad - k_1 \overline{[\text{O}_3]} \overline{[\text{NO}]}. \end{aligned} \quad (8)$$

where the photolysis rate *J_{NO2}* and reaction rate constant *k₁* are temperature-dependent and derived from (Shetter et al., 1988):

$$\begin{aligned} J_{\text{NO}_2} &= 8.14 \times 10^{-3} \left\{ 0.97694 + 8.3700 \times 10^{-4} \times (T - 273.15) \right. \\ &\quad \left. + 4.5173 \times 10^{-6} \times (T - 273.15)^2 \right\}, \end{aligned} \quad (9)$$

$$k_1 = 44.05 \times 10^{-3} \exp \left(-\frac{1370}{T} \right). \quad (10)$$

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