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Review

Coupling dynamics and chemistry in the air pollution modelling of street canyons: A review☆

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ABSTRACT

Air pollutants emitted from vehicles in street canyons may be reactive, undergoing mixing and chemical processing before escaping into the overlying atmosphere. The deterioration of air quality in street canyons occurs due to combined effects of proximate emission sources, dynamical processes (reduced dispersion) and chemical processes (evolution of reactive primary and formation of secondary pollutants). The coupling between dynamics and chemistry plays a major role in determining street canyon air quality, and numerical model approaches to represent this coupling are reviewed in this article. Dynamical processes can be represented by Computational Fluid Dynamics (CFD) techniques. The choice of CFD approach (mainly the Reynolds-Averaged Navier-Stokes (RANS) and Large-Eddy Simulation (LES) models) depends on the computational cost, the accuracy required and hence the application. Simplified parameterisations of the overall integrated effect of dynamics in street canyons provide capability to handle relatively complex chemistry in practical applications. Chemical processes are represented by a chemical mechanism, which describes mathematically the chemical removal and formation of primary and secondary species. Coupling between these aspects needs to accommodate transport, dispersion and chemical reactions for reactive pollutants, especially fast chemical reactions with time scales comparable to or shorter than those of typical turbulent eddies inside the street canyon. Different approaches to dynamical and chemical coupling have varying strengths, costs and levels of accuracy, which must be considered in their use for provision of reference information concerning urban canopy air pollution to stakeholders considering traffic and urban planning policies.

1. Introduction

The terminology "street canyon" typically describes a restricted space in an urban area with surrounding buildings, usually along both sides of a street (Jeong and Andrews, 2002). In such an atmospheric compartment, natural air ventilation through dynamical processes is drastically constrained compared with open space (Cheng et al., 2008). Emissions from vehicles, such as nitrogen oxides (NO_x), carbon monoxide (CO), volatile organic compounds (VOCs) and particulate matter (PM), are predominant among various anthropogenic pollutant sources inside street canyons in urbanised areas. Many such emitted species are reactive (Park et al., 2015), undergoing chemical processing within the street canyon to generate secondary pollutants such as ozone (O_3) and secondary aerosol. The deterioration of air quality in street canyons therefore occurs due to combined effects of the emissions source, dynamical processes (reduced dispersion) and chemical processes (evolution of reactive primary and secondary pollutants) (Li et al., 2008b). The urban canopy is the location in which the majority of outdoor activities of the urban population occurs, and hence where substantial human exposure results for pedestrians, road-users and occupants of adjacent buildings which may gain their ventilation from the outdoor (canyon) environment. Exposure to such environments causes adverse health effects (Solazzo et al., 2011). Since both the primary and secondary pollutants exhibit inhomogeneous distributions in urban street canyons and vary substantially in abundance with time, it is not an easy task to assess individual or population exposure to such air pollutants. The pedestrian level (breathing height) in street canyons is expected to experience particularly high levels of pollutants due to the proximity to vehicle emissions. Pollutant abundance within street canyons frequently far exceeds that in the wider urban background; in 2005, for

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example, measured data at the London Marylebone Road 'supersite' showed that NO_2 hourly concentrations exceeded the hourly objective 853 times compared with 0 exceedances at the nearby London Westminster urban background site (Preen and Neville, 2009). Both short term exposure to high levels of pollutants and long term exposure to lower levels may cause adverse health impacts (WHO, 2000). Air quality objectives, specified for long term averages (hours, days or annual) may be inadequate to account for the exposure associated with the real nonlinear fluctuations in pollutant abundance in urban street canyons, with repeated aperiodic peaks present for short periods. Understanding both dynamic and chemical processes governing the abundance of reactive pollutants in street canyons is of vital importance to accurately quantify personal exposure, and to help urban planners develop policies (e.g. street canyon design and utility of green infrastructure) to mitigate such health impacts.

Various approaches have been undertaken to investigate air pollution in street canyons, such as field measurements, physical modelling, numerical modelling and parametric (operational) modelling. Field measurements can provide first-hand information on pollutant abundance (subject to the limitations of measurement technologies), air flow and pollutant dispersion, and can ground-truth models, but with some limitations (e.g. challenges to data interpretation, uncontrollable meteorological conditions, low spatial coverage, and typically high expense). Physical modelling (e.g. wind tunnels and water channels) only provides insight into dynamics; such approaches are able to fully control testing parameters and sampling points, and to provide well-documented datasets for the evaluation of numerical models. Due to scale limitations, it is a challenge for such models to replicate fully the large-scale atmospheric turbulence of the real world and hence to scale the nonlinear photochemical reactions with a wide range of time scales. Numerical modelling can provide high spatial and temporal distributions of flow and pollutant fields in street canyons, with increasing accuracy and precision compared with the available observations for validation. Such models can be repeated with controllable test parameters at relatively low economic expense. However, they normally require a high level of computational resource and may require substantial input information (computational domain, flow characteristics, chemical schemes). Parametric modelling can provide useful time-series information regarding pollutant abundance for regulatory applications, based on semi-empirical parameterisation of street canyons (and emissions). This approach is relatively simple to use and demands far less computational cost than numerical modelling. However, due to the inherent semi-empirical assumptions, parametric models are unable to reproduce the detailed distribution of the flow or pollutant fields in street canyons.

Recent reviews have provided an overview of specific individual aspects of urban street canyon dynamics or pollution or chemistry. Ahmad et al. (2005) reviewed wind tunnel experiments on wind flow and pollutant dispersion patterns in street canyons. Vardoulakis et al. (2003) examined a range of approaches (from measurements to modelling) for the study of air quality in street canyons, focusing upon measurements and parametric modelling approaches, with little discussion of computational fluid dynamics (CFD) modelling. Subsequently, Li et al. (2006) conducted a separate review on the CFD modelling of wind flow and pollutant transport in street canyons, focusing upon dynamical processes of pollutant dispersion within street canyons, rather than on the chemical processes. Yazid et al. (2014) reviewed a variety of studies (from measurements to modelling) addressing flow structure and pollutant dispersion to provide guidelines for urban planning strategies. While this study briefly considered chemical reactions, there is limited discussion on the coupling of dynamics and chemistry. With ongoing improvements of advanced computer technology, it has become feasible to apply detailed numerical modelling approaches to explore the coupling between dynamical and chemical processes involving pollutant dispersion and transformation in street canyons. The dynamics-chemistry coupling approach has increasingly been applied to the street-canyon scale (e.g. Kwak and Baik, 2014; Zhong et al., 2015), with a range of related, but distinct approaches, and associated advances in our understanding of urban street canyon pollutant abundance. It is in this new context that the present paper reviews progress in the development of coupling between dynamics and chemistry, as applied to street-canyon air pollution modelling, with a focus upon gas-phase processes.

2. Modelling dynamics in street canyons

Street canyon geometry is normally characterised by the aspect ratio, i.e. H/W (building-height-to-street-width, herein referred as to AR) and L/W (building-length-to-street-width). According to Vardoulakis et al. (2003), street canyons might be classified into avenue ($AR \leq 0.5$), regular ($0.5 < AR < 2$) and deep ($AR \geq 2$) street canyons or into short ($L/W \leq 3$), medium ($3 < L/W < 7$) and long street canyons ($L/W \geq 7$). This classification is based on the geometrical detail of a street canyon, which may be empirically derived and widely used. When L is infinitely large, this corresponds to a two-dimensional (2D) street canyon; otherwise, a three-dimensional (3D) street canyon architecture must be considered and the value of L describes the distance between two street intersections. Flow patterns in street canyons under neutral meteorological conditions with perpendicular approaching wind can be classified into three main regimes (Oke, 1987): isolated roughness flow (IRF), wake interference flow (WIF) and skimming flow (SF). The IRF regime is related to widely spaced buildings ($AR < 0.3$). The WIF regime is associated with the closer spaced buildings ($0.3 < AR < 0.7$). The SF regime occurs in more tightly spaced buildings ($AR > 0.7$), representing the worst-case scenario for pollutant dispersion.

2.1. Numerical modelling

As a numerical modelling technique, CFD is a powerful tool to explore experimental flow problems, to characterise air pollutant transport and dispersion processes, and to provide a detailed distribution of canyon flow and pollutant dispersion with high spatial-temporal resolution (Chang, 2006). A CFD package may include a series of numerical governing equations for turbulent flow and pollutant dispersion, potentially involving the coupling of both dynamics and chemistry. The turbulence closure schemes for the CFD packages are classified into two categories: Reynolds-averaged Navier-Stokes (RANS) and Large-Eddy Simulation (LES). RANS resolves only the mean time-averaged properties with all the turbulence motions to be modelled. In place of the time-averaging used in RANS, LES adopts a spatial filtering operation and consequently resolves large-scale eddies directly and parameterises small-scale eddies using sub-grid scale (SGS) turbulence models. In this aspect, the RANS approach is more easily established and computationally faster than LES. The atmospheric turbulent flow in and above street canyons involves turbulent eddies on a variety of scales (Mcnabola et al., 2009). The sizes of large-scale eddies are usually comparable to the characteristic length of atmospheric turbulent flow, and are dependent on the street canyon geometry and turbulent flow boundary conditions. Small-scale eddies typically have a universal behaviour throughout the computational domain and are more dependent on the local energy dissipation. Applications of RANS and LES in street-canyon dynamics are