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Simulating urban air pollution: large-eddy simulation versus an operational model

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Computational modelling of air pollution in the urban microclimate is integral to understanding, and therefore facing, the challenges of air quality in our cities. Yet our ability to accurately model urban pollution dispersion is limited by the complex, heterogeneous and multi-scale nature of the urban environment. Operational models, which are typically used by public authorities and urban planners, utilise detailed morphological, emissions and meteorological data but are limited by their simplified parametrised flow representation (O(100 m, 1 hr)). Whilst large-eddy simulation (LES) models time-resolve the turbulent urban flow field at high resolutions (O(1 m, 0.1 s)) but are typically used in intensive studies of idealised morphologies, inert scalars and neutral conditions.

A systematic case study is therefore conducted into air pollution over South Kensington, London using both the LES model, DALES-Urban (Heus, 2010; Tomas, 2015), and the street-network model, SIRANE (Soulhac, 2011), providing a direct comparison between these two contrasting numerical models. A set of comparable, steady-state simulations are run based on the same fundamental input data utilising both neutral and convective conditions and inert and reactive scalars. Realistic urban morphologies of the case study area are generated using 1 m vector-based LIDAR data and emissions are obtained using the traffic microsimulation model VISSIM (PTV AG, 2017) amalgamated by local traffic counts. The research output provides (1) an unprecedented insight into the role of and interplay between buoyancy and chemistry effects on air quality in the urban microclimate and (2) an evaluation of the predictive skill and parametrisations of SIRANE against the most detailed possible dataset.

On the whole, SIRANE is shown to perform well in predicting canyon-averaged concentrations and velocities, particularly when considering the difference in computational requirements between the two models. Under neutral conditions and with an inert scalar field, SIRANE accurately captures the dominant trends with respect to canyon-averaged concentrations (fractional bias, FB=-0.06 and normalised mean squared error, NMSE=0.08) but exhibits a source of systematic error in regard to the use of uniform in-canyon concentrations to assess pedestrian-level exposure. A linear correction factor, m=1.66, is proposed (and shown to be robust against different street types and angles of incidence) that accounts for this underestimation.

Under neutral conditions and with reactive scalars, SIRANE exhibits an over- and underprediction of NO_2 (FB=-0.23) and O_3 (FB = 0.27) respectively. The assumption of photostationarity is shown to lead to this systematic error with photostationary steady-state defects shown to be as high as 200% close to busy roads in DALES-Urban. Incorporating a chemistry scheme into DALES-Urban significantly altered the resulting spatial distribution of e.g. NO_2 and is shown to be integral to accurately modelling pedestrian-level exposures to NO_2 and O_3.

Results from simulations using convective conditions will also be presented, which explore the effect of buoyancy on urban pollution dispersion and quantify the limitations of SIRANE's parametrisation for accounting for the enhanced vertical exchange of pollutants out of the street-network.