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Estimating the time evolution of urban pollutant concentrations using offline CFD

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ABSTRACT

NO_2, NO_x and $PM_{2.5}$ concentrations within two densely built-up areas are predicted using offline steady-state CFD simulations by adapting the WA CFD-RANS methodology introduced by Parra et al. 2010. Statistical metrics for the pollutants indicate good agreement with a two-week measurement campaign and air quality monitoring data for 2021. The performance is assessed with respect to the assumptions required for pollutant concentrations to be estimated from RANS simulations for different inflow wind directions. It is shown that these assumptions are satisfied by many different configurations over a wide range of meteorological conditions since background concentrations play an important role, the turbulence time scale is short, the impact of wind-direction fluctuations is limited, and the flow is fully developed. Extensive sensitivity testing confirms that good agreement is still obtained for a small set of offline simulations, averaging intervals much shorter or longer than one hour, different definitions of inflow and in situ velocity scales, and substitution of LES for RANS. This work elucidates the conditions under which urban pollutant concentrations can be estimated from offline RANS and demonstrates that the methodology's applicability may extend beyond typical air quality applications.

1. Introduction

A key limitation to the routine use of computational fluid dynamics (CFD) for the prediction of urban winds and air quality is computational cost. This is especially true for applications, such as environmental impact assessment and climatology, which require statistics to be evaluated over a long time interval (e.g. a season or a year). At the present time, transient methods based on large-eddy simulation (LES) or the unsteady Reynolds-Averaged Navier–Stokes (RANS) equations are too computationally expensive for many real-world applications (e.g. Salim et al., 2011; Hadžiabdić et al., 2022). Hence fast dispersion (e.g. Soulhac et al., 2012) or Gaussian puff (e.g. Bonifacio et al., 2014) models are used operationally even though it is widely accepted that the accuracy of CFD is superior to that of theoretical or semi-empirical models.

An interesting and important alternative to direct CFD simulations was introduced by Parra et al. (2010). This methodology, referred to as weighted average CFD-RANS (WA CFD-RANS) by Santiago et al. (2017), predicts time-dependent urban pollutant concentrations from steady RANS simulations by applying a scaling factor based on the ratio of inflow and in situ velocity scales. The great advantage of this method is that it eliminates the need for many RANS simulations with different inflow boundary conditions or a very long simulation with a transient method. Huge computational savings are therefore obtained. For example, Santiago et al.

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