REDUCED-ORDER MODELING FOR PARAMETERIZED LARGE-EDDY SIMULATIONS OF ATMOSPHERIC POLLUTANT DISPERSION

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ABSTRACT

Mapping near-field pollutant concentration is essential to track accidental toxic plume dispersion in urban areas. By solving a large part of the turbulence spectrum, large-eddy simulations (LES) have the potential to accurately represent pollutant concentration spatial variability. Finding a way to synthesize this large amount of information to improve the accuracy of lower-fidelity operational models (e.g. providing better turbulence closure terms) is particularly appealing. This is a challenge in multi-query contexts, where LES become prohibitively costly to deploy to understand how plume flow and tracer dispersion change with various atmospheric and source parameters. To overcome this issue, we propose a non-intrusive reduced-order model combining proper orthogonal decomposition (POD) and Gaussian process regression (GPR) to predict LES field statistics of interest associated with tracer concentrations. GPR hyperpararameters are optimized component-by-component through a maximum a posteriori (MAP) procedure informed by POD. We provide a detailed analysis of the reduced-order model performance on a two-dimensional case study corresponding to a turbulent atmospheric boundary-layer flow over a surface-mounted obstacle. We show that near-source concentration heterogeneities upstream of the obstacle require a large number of POD modes to be well captured. We also show that the component-by-component optimization allows to capture the range of spatial scales in the POD modes, especially the shorter concentration patterns in the high-order modes. The reduced-order model predictions remain acceptable if the learning database is made of at least fifty to hundred LES snapshot providing a first estimation of the required budget to move towards more realistic atmospheric dispersion applications.

***K*eywords** Air pollutant dispersion, Boundary-layer flow, Large-eddy simulation, Parametric uncertainty, Proper orthogonal decomposition, Gaussian process regression

1 Introduction

Accidental short-term pollutant emissions (e.g. 2011 Fukushima power plant explosion – Tsuruta et al., 2014; 2019/2020 Australian bushfires – Graham et al., 2021) can significantly degrade air quality and impact public health. In urban areas, peak pollutant concentrations are difficult to track due to the complex interactions between meteorology and urban topography [Philips et al., 2013]. As a result, predicting the range of possible scenarios for near-source air pollutant dispersion in urban areas is critical for decision support in emergency situations [Da Silva et al., 2021].

Computational fluid dynamics (CFD) is a complementary approach to field campaigns (e.g. Oklahoma City Joint Urban 2003 Experiment – Allwine and Flaherty, 2006) to study microscale atmospheric dispersion processes in a complex urban environment [Tominaga and Stathopoulos, 2013, Dauxois et al., 2021]. CFD has first been tackled through

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