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Quantifying uncertainties in large eddy simulations of pollutant dispersion using surrogate models

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Accurately predicting the unsteady short-to-medium range plume dynamics and dispersion induced by emission source(s) remains a challenge for air quality prediction and health impact quantification. Large eddy simulation has been identified as a promising tool to tackle this challenge. At the scale of micro-meteorology, simulating the near field is a multi-physics multi-scale problem since pollutant concentrations can vary by orders of magnitude in time and space due to the complex flow dynamics induced by the presence of obstacles (e.g. buildings) in a urban district or an industrial site as well as time-transient meteorological conditions. We thus need to analyze how uncertainties affect pollutant concentration predictions. Since large eddy simulations are computationally expensive, we have access to a limited number of simulations. To overcome this issue, we investigate the use of a surrogate model to quantify concentration uncertainties and analyze concentration sensitivity with respect to inlet flow conditions. Two surrogate strategies are compared, Polynomial Chaos and Gaussian Process, in terms of approximation of statistical moments and Sobol'sensitivity indices. The methods will be illustrated in the framework of the MUST (Mock Urban Setting Test) field-scale experiment [1] corresponding to an idealized urban environment. The MUST experiment was simulated using the large eddy simulation code YALES2-AE (CERFACS/CORIA) [2]. An ensemble of 30 large eddy simulations was carried out, each simulation corresponding to a different inlet wind scenario, and form the training set for the surrogate models.

References

[1] Yee, E., Biltoft, C. A., 2004. Concentration fluctuation measurements in a plume dispersing through a regular array of obstacles. Boundary-Layer Meteorology 111 (3), 363–415.
[2] G. Rea, M.C. Rochoux, F. Auguste, O. Vermorel, A. Lopez Gascon & D. Cariolle: Model intercomparison in micro-scale meteorology and pollutant dispersion: large eddy simulations of the MUST experiment, Atmospheric Environment, in preparation.

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