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Adaptive Gaussian process surrogate modelling of large-eddy simulation for microscale atmospheric dispersion

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Mapping pollutant concentration fields at the microscale is essential to track accidental toxic plume dispersion in urban areas but remains a modelling challenge due to complex turbulent flow dynamics. Large-eddy simulations (LES) are well suited to capture such dynamics. However, their responses are far from real time, come with high-dimensionality and do not efficiently handle atmospheric dispersion intrinsic uncertainties. For instance, these uncertainties are associated with large-scale meteorological forcing and pollutant source characteristics. Therefore, extracting the main features from LES data and designing surrogate models that both incorporate physical information from LES and account for uncertainties could make a shift in emergency planning and response in the long term [1,2].

In the present work, we have designed an efficient two-step statistical procedure for emulating high-dimensional turbulent flow information provided by LES: *(i)* the main features from the time-averaged tracer concentration fields are extracted using proper orthogonal decomposition (POD); and *(ii)* a surrogate model representing the dependence of the first POD modes to the uncertain parameters is trained. We have completed a proof-of-concept study on a simplified but representative flow configuration (2-D flow around a surface-mounted obstacle) using the *AVBP* LES code with a broad LES dataset (of the order of a few hundreds). We carried out an exhaustive surrogate-to-surrogate comparison involving state-of-the-art learning techniques, *e.g.* polynomial chaos, Gaussian process, random forest and gradient boosting. An adaptive procedure optimizing Gaussian process' correlation length scales with respect to each POD mode demonstrated better performance results. Future work includes applying the adaptive Gaussian process surrogate model to more realistic cases such as the MUST (Mock Urban Setting Test) field campaign.

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