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SENSITIVITY ANALYSIS OF MICROSCALE POLLUTANT DISPERSION LARGE-EDDY SIMULATIONS TOWARDS OBSERVATION NETWORK DESIGN

Eliott Lumet[1,2], Mélanie C. Rochoux[1], Simon Lacroix[2], Thomas Jaravel[1] and Olivier Vermorel[3]

[1]CECI, Université de Toulouse, CNRS, CERFACS, Toulouse, France
[2]LAAS-CNRS, Toulouse, France
[3]CERFACS, Toulouse, France

Abstract: We present a detailed study of the influence of the atmospheric boundary-layer variability on large-eddy simulation (LES) model predictions in the context of microscale pollutant dispersion in urban-like environments. For this purpose, we have developed a new approach to model inflow boundary conditions and their related uncertainties that are essential to represent how the large atmospheric scales influence the microscale flow features in a complex urban geometry. In a preliminary step, we have considered uncertainties in the inflow mean wind direction and in the friction velocity of the mean wind velocity logarithmic profile. We have then built a perturbed-physics ensemble of tracer concentration fields by integration of the LES model in a multi-query framework. In this study, the ensemble of LES fields is obtained for the Mock Urban Setting Test (MUST) field-scale experiment and it is used to carry out a global sensitivity analysis, i.e. to quantify the LES model spatial dependencies to the mean wind direction and the friction velocity.

Key words: *Microscale dispersion, MUST, Large-Eddy Simulation, Inflow boundary conditions, Sensitivity Analysis*

INTRODUCTION

Large-eddy simulations (LES) are a promising approach to simulate microscale meteorology and pollutant dispersion in complex urban environments, since they can accurately capture highly unsteady and complex flow topologies typically found in the wake of buildings, and thereby track the spatiotemporal variability of pollutant concentration in urban canopies. This is of primary importance to capture the peak pollutant concentrations for instance (Philips et al. 2013). However, to correctly predict microscale pollutant dispersion in complex geometry, LES models have to account for the variability of the atmospheric boundary-layer and in particular for the complex interactions with the turbulence mesoscales (Nagel et al. 2022). For this purpose, boundary conditions models can be used, but their parameters are highly uncertain and it is therefore advised to adopt a probabilistic representation of the boundary conditions to reflect their uncertainties (Dauxois et al. 2021). In this context, we aim at applying data assimilation methods to LES dispersion models, i.e. at solving an inverse problem that combines LES model predictions with in situ measurements to infer more accurate inflow boundary conditions (Defforge et al. 2021). It is therefore of primary importance to identify where to place sensors to extract the most informative data and thus have a well-posed data assimilation problem (Peng et al 2014). To design the observation network, a preliminary step consists in carrying out a sensitivity analysis to spot which areas are subject to high uncertainties in the LES predictions, and thereby determine in which areas potential sensors could be used to reconstruct information on the uncertain inflow boundary condition. In this study, this approach has been applied to one near-neutral trial of the Mock Urban Setting Test (MUST) experiment, which is a good validation case for the LES simulations (Yee and Biltoft, 2004) and which is used here to provide a proof of concept of the proposed sensitivity analysis approach.

THE MUST (MOCK URBAN SETTING TEST) CASE

The experiment

MUST is a field-scale experiment performed in September 2001 in Utah, USA, to provide extensive measurements of pollutant dispersion within an urban-like canopy for model development and validation purpose (Yee and Biltoft, 2004). The simplified urban canopy is represented by an array of 120 regularly-spaced shipping containers disposed over a flat and homogeneous terrain. Each container measures 12.2 m long, 2.42 m wide and 2.54 m high. A series of trials was performed for which a non-reactive gas, propylene, was released under different atmospheric conditions during 15 minutes. For this study, we simulate the trial 2681829 corresponding to near-neutral atmospheric conditions since it has been extensively studied in the literature (it is of particular interest to study the container impact on the incident flow within the container array) and is therefore a relevant validation test case for our modeling approach.

The large-eddy simulation solver and related modeling choices

To reproduce the MUST case, we design and run obstacle-resolved LES to predict the temporal evolution of the flow and the propylene transport across the container array. For this purpose, we use the AVBP solver developed by CERFACS (https://www.cerfacs.fr/avbp7x) which solves the filtered compressible Navier-Stokes equations on unstructured meshes using a finite volume discretization and the second-order in time and space Lax-Wendroff scheme. Since the Mach number of atmospheric boundary-layer flows is very low, an artificial compressibility approach, also known as pressure gradient scaling, is used to artificially increase the time-step and thereby reduce the computational time.

The computational domain is a square box of size $L \times l \times h = 420\ \mathrm{m} \times 420\ \mathrm{m} \times 50\ \mathrm{m}$ (Fig. 1). It is discretized based on an unstructured tetrahedral mesh of $14{,}7 \times 10^6$ cells, with refinement in area of interest and towards walls, down to 30 cm resolution at the obstacles level. To efficiently handle changes in the mean inflow direction, the computational domain is separated in two subdomains (Fig. 1): the peripheric domain D2 that is turned to align with the mean inflow direction, and the inner domain D1 that is fixed. We solve the Navier-Stokes equations on all subdomains using the coupling library CWIPI. This is useful to avoid generating a new mesh for each new set of input parameters and facilitate the generation of a large ensemble of LES runs.

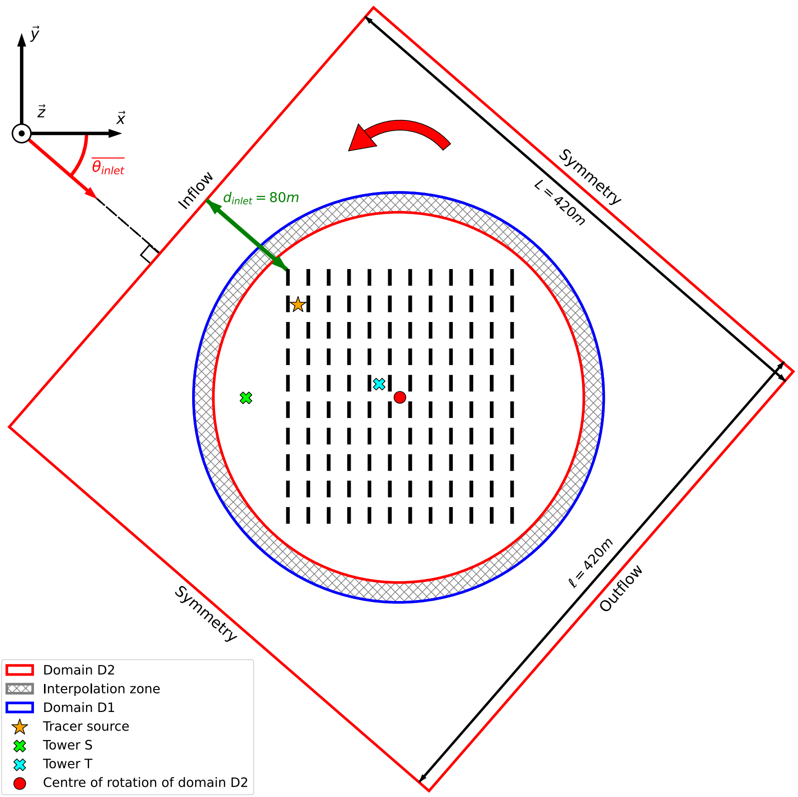

Figure 1. Schematic of the simulation subdomains D1 and D2 for the simulated MUST trial using LES: the fixed inner domain is in blue, the rotating peripheric domain D2 is in red, and the overlap area between D1 and D2 is hatched. Lateral boundary conditions are indicated. The orange star represents the emission source location. The cross symbols represent the towers at which observations were acquired during the trial: the upstream tower S is indicated in green, while the inner tower T is indicated in blue.

A mean wind log-law vertical profile (Eq. 1) is imposed at the inlet based on the Monin-Obukhov similarity theory in neutral atmospheric conditions:

$$\overline{U(z)} = \frac{u_*}{\kappa} \ln\left(\frac{z+z_0}{z_0}\right). \quad (1)$$

This profile was fitted with the experimental data obtained at Tower S (Fig. 1), which is located upstream of the container array. Wind fluctuations are added to the mean inlet wind profile using the Kraichnan synthetic injection method following the Passot-Pouquet turbulence spectrum (Daviller et al. 2019). In this study, we impose a prescribed mean vertical profile of the Reynolds tensor obtained from a free-field precursor simulation of the atmospheric boundary-layer. This novel approach provides a way to have inhomogeneous anisotropic inflow boundary conditions and only requires to know the friction velocity u_*, the ground rugosity z_0 and the mean wind direction $\overline{\theta_{inlet}}$ to parametrize inflow turbulence. In complement to the inlet, wall laws with adapted roughness are used for the ground and the buildings, outflow boundary conditions are used for the outlet and top boundaries, while symmetry is imposed on the domain sides (Fig. 1). Propylene is released as a passive gas tracer from a continuous and constant point source emission.

GLOBAL SENSITIVITY ANALYSIS FRAMEWORK

The key idea of global sensitivity analysis in this context is to quantify how uncertainties in each input parameter influence the variance of a given quantity of interest in the LES model. This is useful to spot the most influential parameters on the LES model response across the computational domain. A preliminary One-At-a-Time (OAT) sensitivity analysis showed that perturbations of the ground roughness length z_0 and of the inflow turbulent kinetic energy parameter do not significantly impact the simulated mean fields of interest comparatively with the atmospheric boundary-layer intrinsic variability. We also assume that the emission source parameters, position and intensity, are known. The sensitivity analysis is therefore restricted to the two inflow parameters that have the strongest impact on the LES predictions: the friction velocity u_* that drives the mean inflow profile (Eq. 1), and the mean inlet wind direction $\overline{\theta_{inlet}}$.

Parameter space sampling

The range of variation of the two uncertain parameters is defined from a climatology obtained in the vicinity of the MUST area. Wind statistics were computed based on 12 days of meteorological measurements from the station SAMS #08 located 1600 m southeast of the obstacles (Yee and Biltoft, 2004). According to these statistics, most of the wind velocity magnitude measurements at 10-m AGL are between 0 and $12\ \mathrm{m\ s^{-1}}$. To avoid complications with very low wind speed, we limit the range to [1; 12 $\mathrm{m.s^{-1}}$]. We can also note that no wind direction prevails. Since it is a preliminary study and to reduce the computational cost associated with the parameter space sampling, we limit the wind angle to a variation of $\pm 30°$ from the North direction. The mean wind angle of $-40.95°$ recorded at the upstream Tower S (Fig. 1) is included in this interval $[-60°, 0°]$ expressed in the MUST frame of reference.
Once the range of variation of the parameters is defined, the next step is to choose for which values of the parameters the LES model is run to generate the ensemble. Since the LES model is very computationally expensive, it is not possible to have a very large sample (our budget is limited to 100 runs) but still we need to have a good coverage of the uncertain space to capture well the LES model response. We therefore use the Halton's low-discrepancy sequence to homogeneously sample the input parameter space (Fig. 2).

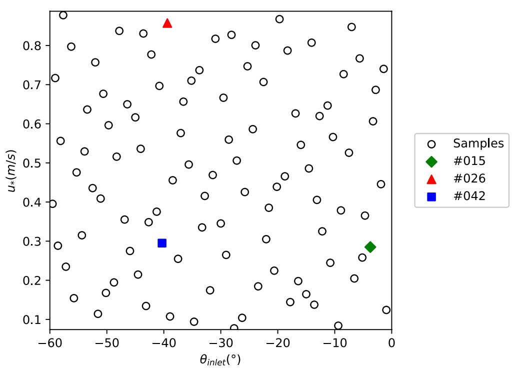

Figure 2. Parameter space sampling obtained with the Halton's low-discrepancy sequence with the inlet wind direction in the *x*-axis and the friction velocity in the *y*-axis: each point is a pair of parameters for which a LES is run.

The LES model is then integrated for each sample parameters of the Halton's sequence. It simulates unsteady flow and tracer concentration fields across the domain from which time-averaged statistics can be derived. For validation, we compare LES averages over a 200-s time period after a spin-up with experimental data acquired over the [300 s; 500 s] time period of the trial 2681829 following recommendations by Yee and Biltoft (2004). Note that the spin-up duration is scaled by the friction velocity because when the wind speed is slow, the plume takes longer to establish. The Reynolds tensor profile prescribed for the turbulence injection is also scaled by u_* and rotated to align with $\overline{\theta_{inlet}}$.

Sobol' sensitivity indices

To study the sensitivities of our LES model to the mean inlet wind direction and friction velocity, we estimate the first-order Sobol indices S_i using the Monte Carlo method from Saltelli (2002). These indices give the share of total model variance, for one field Y, explained by each input parameter X_i (Eq. 2):

$$S_i = \frac{\mathbb{V}(\mathbb{E}(Y|X_i))}{\mathbb{V}(Y)}. \tag{2}$$

These indices vary between 0 and 1, 1 meaning that 100% of the LES model variance is due to the standalone ith parameter. This analysis is performed for each node of a specific analysis grid defined as a 1-m resolution horizontal cut of the D1 domain at a height of 1.6 m. To limit the cost of the Saltelli method, we use a Radial Basis Function (RBF) to interpolate the LES model predictions between the samples from the Halton's sequence. The RBF model was validated and its hyperparameters (kernel model, number of neighbors, etc) were optimized by splitting the Halton's sequence sample into a training set (80 members) and a validation set (20 members), leading to a mean absolute error of 0.189 ppm. Tests showed that a Saltelli's sequence of 2048 samples was enough to have converged estimated Sobol' indices.

RESULTS

The effect of the input parameter perturbations on the plume shape is highlighted by comparing the 1 ppm-isolines of the (time-averaged) mean tracer concentration fields obtained for three ensemble members of the Halton's sequence (Fig. 3); these members are representative of the variety of the LES model response in this study. As expected, when the friction velocity increases, the plume is shorter, while the plume centerline remains the same. The wind inlet direction has more impact since it deflects the plume centerline and can significantly change the flow-obstacle interactions.

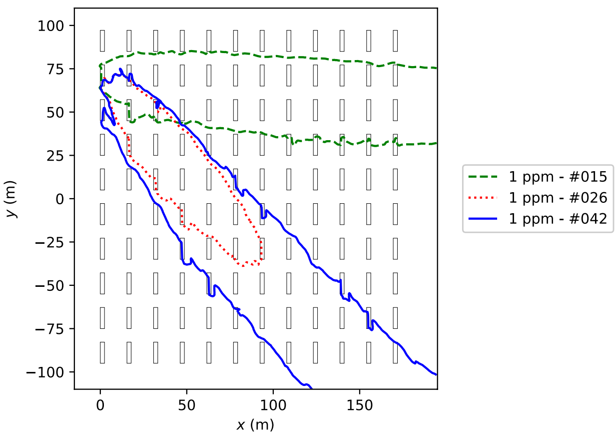

Figure 3. Comparison of the 1 ppm-isoline at $z = 1.6$ m predicted by the LES simulations corresponding to the Halton sample #015 in green, #026 in red, and #042 in blue. The corresponding input parameters are shown in Fig. 2.

The first-order Sobol indices (Eq. 2) are estimated for the horizontal cut at $z = 1.6$ m of the mean tracer concentration field. We thereby obtain 2-D maps of Sobol' indices (Fig. 4), which demonstrate that there are spatially organized patterns of concentration dependency to the inflow boundary conditions parameters in our LES model. The sides of the ensemble-averaged plume centerline are mainly dependent on the inflow wind direction (the yellow-to-orange areas on the left panel of Fig. 4) as these regions are crossed by the plume only for some extreme wind direction values. On the contrary, the concentration in the near source region appears to be mainly driven by the wind velocity (the yellow-to-orange areas on the right panel of Fig. 4). There is also a region where both wind velocity and wind direction have a more equal contribution to the tracer concentration (the pink-to-purple areas in Fig. 4); this is related to the plume size associated with the ensemble mean. These sensitivity maps are clearly useful from an experimental design perspective, as they tell us where the sensors would be able to catch perturbations information on the wind boundary conditions in a data assimilation framework.

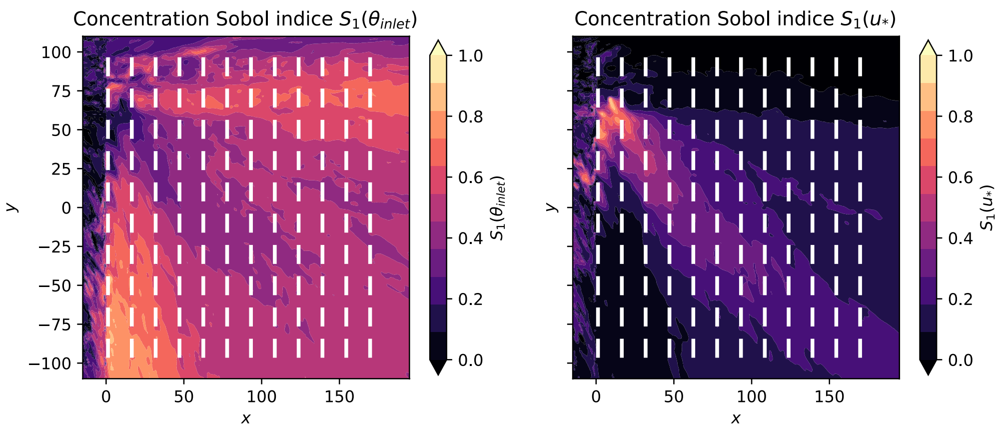

Figure 4. First-order Sobol indices of the mean concentration field at $z = 1.6$ m with respect to the mean inlet wind direction (left) and to the prescribed friction velocity (right).

CONCLUSION

To investigate the LES model sensitivities to the wind boundary conditions in the context of microscale dispersion, we designed and built a perturbed-physics ensemble of LES for a near-neutral trial of the MUST field campaign. From a modeling viewpoint, a particular focus has been on the development of inflow boundary conditions representative of atmospheric boundary-layer turbulence using a synthetic injection method combined with free-field precursor simulation to impose anisotropic vertical wind profiles at the boundary conditions. From a stochastic viewpoint, the LES model response (i.e. the relationship between the 2-D mean tracer concentration field at the human level and the wind direction and friction velocity) was studied using Sobol' indices. This allows to identify which regions of the microscale domain are the most sensitive to the wind direction and/or to the friction velocity. Future work includes replacing the RBF simple interpolation by a more robust metamodel based on machine learning to increase representativeness of the sensitivity analysis. This will pave the way towards designing a data assimilation framework to estimate the uncertain inflow parameters by aggregating surrogate model predictions with in-situ measurements. To go further, we will investigate how we can use the spatial distribution of the LES model sensitivities to provide guidelines to optimize the sensors' locations so as to improve data assimilation performance.

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