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MODITIC- ON THE GENERATION OF INFLOW BOUNDARY CONDITIONS FOR DISPERSION SIMULATIONS USING LARGE EDDY SIMULATIONS.

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Abstract: Development of realistic inflow conditions is crucial to successful use of Large Eddy Simulations in dispersion simulations. In this paper, three different strategies for the development of inflow conditions are presented, and the resulting turbulent statistics for each method are presented and discussed in relation to wind-tunnel experiments conducted at Laboratoire de Méchanique de Lille, and a set of urban dispersion experiments conducted in the MODITIC project. The POD-LSE method is found to give a realistic high Reynolds number turbulent boundary layer, but is not readily applied to arbitrary geometries. For reproducing the flow-field in the urban dispersion wind tunnel experiments, a precursor simulation with a numerical mesh that included the roughness elements used in the experiments was found to be a suitable method.

Key words: *MODITIC, Computational Fluid Dynamics, Large Eddy Simulations, Inflow conditions, Proper Orthogonal Decomposition, Linear Stochastic Estimation*

INTRODUCTION

Computational fluid dynamics methods can be used to accurately describe the dispersion of aerosols and neutral gases in urban environments. The case of urban dispersion of neutrally buoyant gas has been investigated quite extensively in the past, see e.g. Liu et al (2011) and the reviews by Tominaga and Stathopoulos (2013) and Lateb et al. (2016). The case of urban dispersion of a non-neutrally buoyant gas is significantly more difficult, and requires sophisticated models that include the two-way dynamic coupling between the gas-phase and the air flow field. Large Eddy Simulations (LES) are potentially able to accurately account for this two-way coupling, but have the disadvantage of sometimes being overwhelmingly computationally expensive. However, LES can be put to good use by providing detailed data-bases that can serve as a basis for improved understanding of the complex physical processes governing the dispersion of non-neutral gases. These data-bases can also be used in combination with fast operational models for specific geometries, i.e. cities or industrial locations, where the dispersion of gas from a specific location can be predicted rapidly using pre-computed wind-fields from LES, such as e.g. the CT-analyst framework (Boris et al, 2010).

The usefulness of LES can however partly diminish due to unknown or inconsistent inflow boundary conditions. In order to minimize the effect of inappropriate inflow boundary conditions, excessively large computational domains or precursor simulations are often used. These methods significantly increase the computational cost and alternatives are sought. Here, three different approaches for generating inflow conditions for dispersion simulations using LES performed at the Norwegian Defence Research Establishment (FFI) within the MODITIC project (EDA project B-1097-ESM4-GP) are presented and discussed. This project investigated the dispersion of neutral and non-neutral gas in urban environments using both with tunnel experiments and numerical simulations. First a method applying proper orthogonal decomposition (POD) together with linear stochastic estimation (LSE) is presented. In the next section, results obtained with a synthetic turbulence method are presented. This method generates random velocity fluctuations with given statistical properties and these are superimposed onto a known mean flow. Lastly the advantages of using precursor simulations are discussed, and results from two precursor simulations are presented. Throughout this paper u, v, and w denote the streamwise, spanwise and wall-normal fluctuating velocity components respectively.

POD-LSE

Proper orthogonal decomposition is a method which decomposes a given field into a set of orthogonal modes with the property that for any finite number of modes N, the set of N modes used is the set that minimizes the difference between the original field and the reconstructed field. The method was first used in turbulence analysis by Lumley (1967) for identifying dynamical structures with finite energy. In the present study, POD was used on particle image velocimetry (PIV) data from a high Reynolds number turbulent boundary layer experiment conducted at LML (Laboratoire de Méchanique de Lille, France). This experiment was conducted in a wind tunnel with a 20 m long test section and a cross-section of 1x2 m. The free-stream velocity was 10 m/s, and the resulting boundary layer had a momentum thickness Reynolds number of 19100. The boundary layer thickness at the measurement position was δ =30. The application of classical POD on a two-dimensional velocity field gives the following formulation:

$$\int_D R_{ij}\left(y, y', z, z'\right) \phi_j^{(n)}\left(y', z'\right) = \lambda^{(n)} \phi_i^{(n)}\left(y, z\right) \tag{1}$$

where the kernel R_{ij} is the two-point cross-correlation tensor of the fluctuating velocity field:

$$R_{ij} = \langle u_i (y, z) u_j (y', z') \rangle \tag{2}$$

where < > represents an ensemble average, here defined as the average over the ensemble of PIV-planes measured in the experiment.

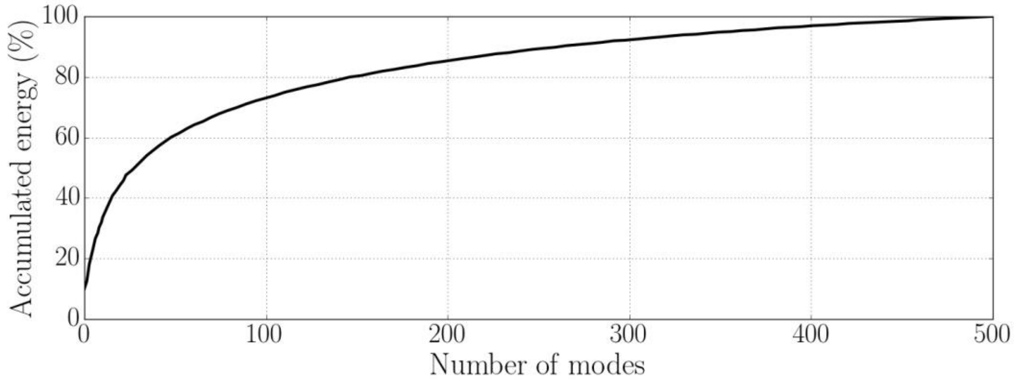

Figure 1. Accumulative content of energy in the POD modes, in %, as a function of number of modes.

Wingstedt et al. (2013) used linear stochastic estimation in combination with POD to construct a velocity field which was highly resolved in both space and time. The PIV-planes, which were highly resolved in space but poorly resolved in time, was combined with hot-wire data, which were poorly resolved in space but highly resolved in time, and a velocity field was constructed based on these. This method also enables reconstruction of a velocity field based on a smaller number of modes while retaining most of the energy in the flow field. The energy content as a function of number of modes is shown in Figure 1. As can be seen, the accumulative energy rapidly increases for the first modes and then flattens as the number of modes increases.

Using this method for generating the inflow boundary condition, a number of turbulent boundary layer simulations were performed. All simulations discussed here were performed with the node-based finite volume incompressible flow solver "Cliff" from Cascade Technologies Inc. (CTI, 2014). Velocity fields with varying amounts of energy were constructed by varying the number of POD-modes, and for each constructed velocity field, a turbulent boundary layer simulation was performed. The numerical simulations used a domain of size 3x0.6x0.3 m in the streamwise, wall-normal and spanwise directions respectively. The number of cells in each direction were 1000, 150 and 100 and the cells were uniformly distributed in the streamwise and spanwise directions. In the wall-normal direction, geometric stretching of the cells was used to obtain a finer spatial resolution close to the wall. The reconstructed velocity field did not cover the entire inlet-plane, missing a small area close to the wall and an area above the boundary layer. In these areas the velocity field was extended by interpolating between zero velocity at the wall and the experimental points closest to the wall, and a constant velocity above the boundary layer.

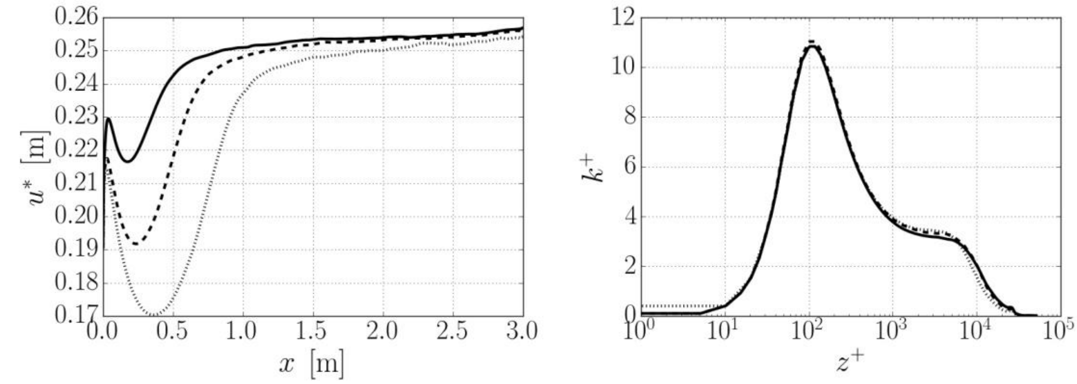

Figure 2. Left: Friction velocity throughout the domain. Right: Turbulent kinetic energy for the turbulent boundary layer simulations with varying inflow energy (in wall units). Solid lines: 100% energy, dashed lines: 75% energy, dotted lines: 50% energy.

The friction velocities obtained from these simulations are shown in Figure 2. As can be seen, the friction velocities have a region close to the inlet where they change rapidly as functions of downstream distance x, but they eventually stabilize to almost the same value for all three configurations. The turbulent kinetic energy at the end of the computational domain is also shown in Figure 2. The resulting peak and plateau structure of the turbulent kinetic energy is characteristic of high Reynolds number turbulent boundary layers. As can be seen, the profiles collapse to almost identical forms when scaled by wall units, indicating that a similar flow field is achieved using all three inflow energies.

SYNTETHIC TURBULENCE INFLOW

As the POD-LSE method generates approximated velocity fields based on a given original field, it is not readily applicable to applications where a velocity field is not known both in space and time. The extension to other geometries and scales is also not straightforward. For this reason, it was not applied to the urban dispersion simulations performed at FFI within the MODITIC project. Instead, a turbulent velocity field was approximated by a random-field generation method in which turbulence scales are prescribed and fluctuations are superimposed on a known mean velocity field. This field was subsequently used as the inlet boundary condition for the LES. This method can be applied directly to a dispersion simulation, but can also be used as input to precursor simulations, as discussed below. A problem with this method is that the constructed velocity field is not generally a solution to the LES equations themselves on the specific numerical grid used. Because of this, when the reconstructed velocity field is used as inflow, there is a region between the inlet and some point downstream where the velocity field is adjusting to the mesh, similar to the initial region in Figure 2. This region is typically long, especially if the spectral content is not realistic (Keating, 2004), e.g. if random noise is used for the velocity fluctuations. Because it is preferred that the interesting region in the simulation is located outside the initial adjustment region, the direct use of synthetic turbulence inflow can be very computationally expensive. A simulation was performed, where a synthetic inflow method was applied by prescribing the Reynolds stress profiles along with the mean velocity profiles measured in the wind-tunnel experiments performed at the Environmental Flow Research Centre in Surrey, within the MODITIC project. This simulation used a computational domain of 10x3.5x1.5 m with 140, 280, and 101 cells in the streamwise, wall-normal and spanwise directions, respectively. Geometric stretching of cells was used in the wall-normal direction. Figure 3 shows Reynolds stress profiles at the end of the domain and the friction velocity throughout the domain. As can be seen, the Reynolds stresses do not agree very well with the experimental values, and are closer to the profiles that correspond to a flat-plate boundary layer. The friction velocity, also shown shown in Figure 3, can be seen to stabilise after about 2 m, which is comparable to the length of the adjustment region obtained with the POD-LSE method, when scaled by the boundary layer thickness (here 1.0 m).

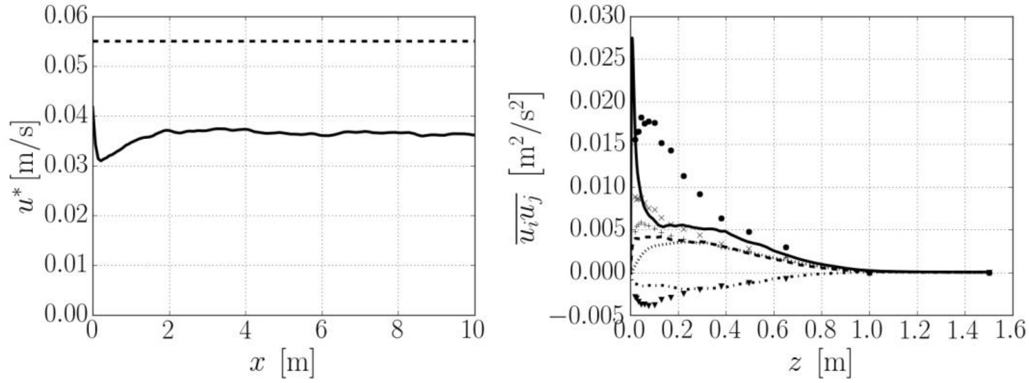

Figure 3. Left: friction velocity throughout the domain. Right: Reynolds stress profiles in the flat plate turbulent boundary layer simulation with synthetic turbulence inflow. Solid line: uu, dashed line: vv, dotted line: ww, dash-dotted line: uw. Symbols indicate the experimental values, • : uu, ×: vv, +: ww, ▼: uw.

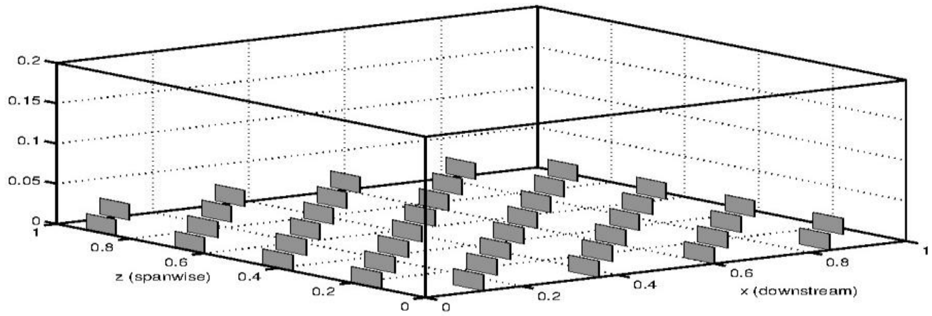

Figure 4. Sketch of the roughness elements used in the precursor simulation and their relative configuration.

USING THE METHOD OF PRECURSOR SIMULATIONS

Using synthetic turbulence as inflow conditions directly to a dispersion simulation significantly increases the computational cost due to the need for an initial and quite large adjustment region that computationally needs to be resolved. A precursor simulation can be suitable, especially when the same inflow can be used for multiple simulations. This was the case in the MODITIC project, where release of neutral and non-neutral gas from different source locations and with different geometries were considered. Most of the wind tunnel experiments used the same upstream turbulent boundary layer and therefore the precursor simulation method was suitable. Two different precursor simulations were performed. One simulation on a flat-plate geometry, as discussed above, and one simulation with roughness elements. The flat-plate precursor simulation was used to obtain the final inflow for simulations of dispersion over the MODITIC hill performed at FFI.

Precursor simulation with roughness elements

The synthetically generated turbulence inflow conditions considered above did not provide Reynolds stress profiles that corresponded well to the experimental results. For this reason, a precursor simulation was performed, where roughness elements, consisting of thin plates, were placed onto the floor. These roughness elements correspond geometrically to the ones used in the wind tunnel. A sketch of the roughness elements and their configuration is shown in Figure 4. The total number of cells in the computational mesh used here was 10^7. As inflow conditions for the precursor simulation the synthetic turbulence method was used. Figure 5 shows the Reynolds stress profiles obtained just before the last row of roughness elements in this simulation. As can be seen, they are in much better agreement with the experimental results than those obtained with the flat-plate precursor simulation. The velocity field obtained with this method was used as inflow for all the dispersion simulations performed at FFI within the MODITIC project, except those with the hill geometry.

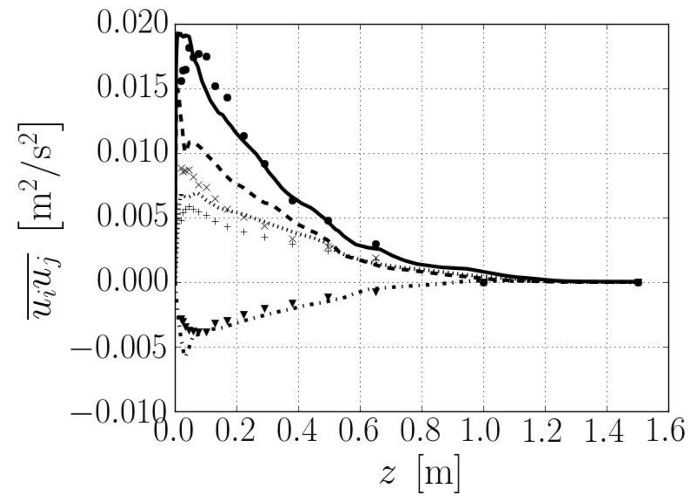

Figure 5. Reynolds stress profiles in the roughness boundary layer simulation with synthetic turbulence inflow. Solid line: uu, dashed line: vv, dotted line: ww, dash-dotted line: uw. Symbols indicate the experimental values, • : uu, ×: vv, +: ww, ▼: uw.

CONCLUSIONS

Three methods for generating time-varying inflow conditions for dispersion simulations using LES have been evaluated. The POD-LSE method was shown to give results that correspond very well to the high Reynolds number turbulent boundary layer upon which the POD field was based, and did not require a long initial adjustment region. However, the method is not readily applicable to arbitrary geometries, and was therefore not used for any dispersion simulations within the MODITIC project. The synthetic inflow method was used for generating inflow for two different precursor simulations, which were subsequently used as inflow for the dispersion simulations performed at FFI. Of the precursor simulations, the roughness element simulation gave results in best agreement with the experimental flow field, and therefore the velocity field from this simulation was used as inflow for most of the dispersion simulations.

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