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SYNTHETIC BOUNDARY CONDITIONS USING LES FOR URBAN DISPERSION MODELLING

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Abstract: Large Eddy Simulation with two sub-grid-scale models are used to simulate gas dispersion, utilizing alternatively constant values and synthetic turbulence at inflow boundaries. The results are compared with data from the JU2003 Atmospheric Dispersion Study in Oklahoma City. Turbulence statistics of the simulation is presented at two probe locations, one inside the city-core and one outside. In addition, comparisons with the measured concentration-data and maximum-values are conducted. It was found that in the core of the city, modeled turbulence is mainly determined by buildings and their configurations, and is only weakly affected by model type and assumed turbulence at inflow boundaries. Within the predicted flow-path, the tested models produce similar predictions of maximum concentration values, which in turn are similar to the experimental data. The results indicate that synthetic turbulence at the inflow boundary is less important when building generated turbulence dominate but it is important if not a local boundary layer is developed.

Key words: *gas dispersion; urban area; LES; CFD; flow statistics; contaminant statistics; JU2003.*

INTRODUCTION

To evaluate the consequences of gas dispersion in a city center, it may be necessary to predict spatiotemporal fluctuations since, for many toxic gases, acute poisoning occurs during the first concentration peak which typically has duration of less than 1 min. However, due to their stochastic nature, single real eddies could hardly be predicted. Specifically, large local variations exist and in a short time interval, i.e., less than a couple of minutes, the concentration vary widely. Correspondingly, Liu et al. (2011) analyzed fluctuations around a high-rise building in wind-tunnel experiments, and found that variations in fluctuation intensity are quite sensitive to both source location and wind direction. Therefore, in order to analyze the consequences of hazardous gas dispersion, a trend exists in which increasingly complex CFD models, including Large Eddy Simulation (LES), are utilized to describe intermittency and fluctuations in wind and concentration fields. It is then necessary to analyze and compare results produced by typical LES Sub-Grid-Scale (SGS) models that might be employed for applied dispersion simulations in urban areas, and determine how these results compare with full-scale experiments.

The scope of the present study is to investigate the usefulness of gas dispersion results for such models by modeling the IOP2 continuous release experiment from the Joint Urban 2003 Atmospheric Dispersion Study in Oklahoma City 2003 (JU2003) using both constant and dynamic settings for turbulence at the inflow boundaries. Two typical LES SGS-models were chosen: 1) the standard static Smagorinsky model and 2) the SIGMA model. In order to investigate the influence of boundary conditions (BC) on important parameters, a dynamic setting for turbulence at the inflow boundaries was examined using the SIGMA model.

MODELING

In this investigation, the transport and diffusion of dispersed gas are modeled according to Patankar (1980):

$$\frac{\partial}{\partial t}(\rho\varphi)+\frac{\partial}{\partial x_i}(\rho\varphi u_i)=\frac{\partial}{\partial x_i}(\Gamma_\varphi\frac{\partial\varphi}{\partial x_i})+S_\varphi \quad (1)$$

where the first term expresses the rate of change of ϕ with respect to time; the second term expresses convection (transport due to fluid-flow); and the third term expresses diffusion (transport due to the variation of ϕ from point to point), where Γ_ϕ is the exchange coefficient of the entity ϕ in the phase. The fourth term expresses source terms (associated with the creation or destruction of ϕ).

In this study two models based on the eddy-viscosity concept have been employed to illustrate the results of the model approaches the , standard Smagorinsky model which is known to be too dissipative in near wall regions (Pope, 2000) and the SIGMA model proposed by Nicoud et al. (2011) which possesses the property that the SGS-viscosity is always positive, it decays as the distance to a solid boundary to the third power, and it vanishes in pure shear as well as in a flow in solid rotation and also has the property that the SGS-viscosity is zero where the resolved scales are either in pure axisymmetric or isotropic expansion/contraction, as well as for any two dimensional and/or two component flows. SGS-viscosity is expressed as:

$$\nu_{SGS_m}=(C_m\Delta)^2 D_m(\vec{u}) \quad (2)$$

for the SIGMA model, D_m is defined as:

$$D_m=\frac{\sigma_3(\sigma_1-\sigma_2)(\sigma_2-\sigma_3)}{\sigma_1^2} \quad (3)$$

where σ_i are the singular values of the tensor G_{ij}, i.e., the appropriately ordered square-roots $(\sigma_1\geq\sigma_2\geq\sigma_3\geq 0)$ of the eigenvalues of $G_{ij}=\Delta^2\overline{A_{ik}}\,\overline{A_{jk}}$. and $\overline{A_{ij}}=\partial\overline{u_i}/\partial x_j$,

The numerical filter width used (Δ) is the cubic root of the cell volume for both models. The Smagorinsky model applies wall damping according to Van-Driest (1956) to partially take wall effects into account by appropriately reducing the length scale in the proximity of walls. The Smagorinsky constant was set to 0.1. In this investigation, in the cases of simulations where inlet fluctuations are used, synthesized inlet fluctuations using Fourier series are applied, according to a method that was first established for generating noise, and later developed for inflow boundary conditions (Davidson, 2007).

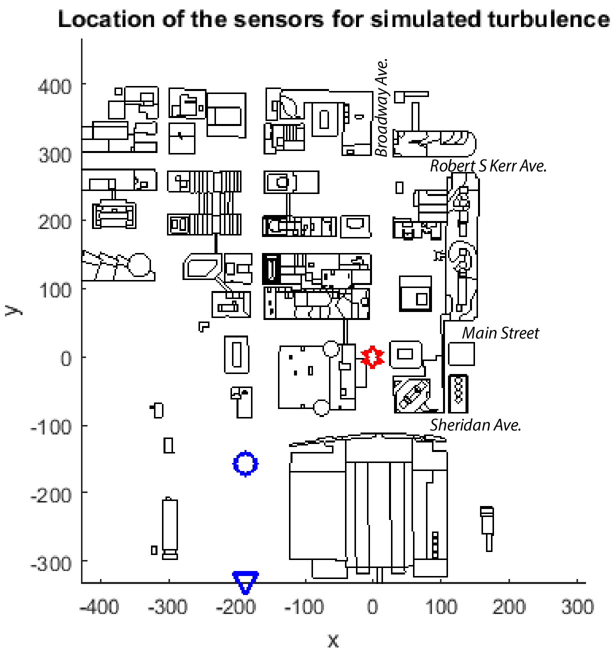


Figure 1. The locations where the simulated turbulence is evaluated. The red star is the location of the source in the IOP2 experiment, and also the probe location in the 'high dense building area' for evaluation of energy spectra. The blue circle is the probe location for the 'low sparse building area'. Hight of the probe is 1.5 m. Blue triangle is the location of the probe for the synthetic turbulence at the inlet boundary

The domain mimics the urban environment from the JU2003 IOP2 experiment, in Oklahoma City, as shown in Figure 1. The grid is cartesian with dimensions of 800 x 850 x 300 m, and includes 218 x 272 x 100 cells. Individual expansion ratios ≤ 1.1 are used. The cell size in the streets are ~1 m wide. Xie and Castro (2009) demonstrated that full-scale resolution of approximately 1 m is sufficient to provide a reasonable estimation of concentration fluctuations. One of the purposes of the survey is to investigate if, and to what extent synthetic boundary conditions can replace extension of the domain when performing applied studies. Finite volume discretization is used to solve the equations with 2nd order convective schemes and 3rd order temporal scheme.Wall functions are used at the surfaces.

Start of evaluation for all flow variables and spectra begins at 60 seconds of simulation when the properties set at the inlet boundary has passed the release point at the roof top height and thereby may influences the vertical dispersion (Hertwig, 2013). At the ground level, the urban boundary layer turbulence dominates the dispersion.

RESULTS

Turbulence

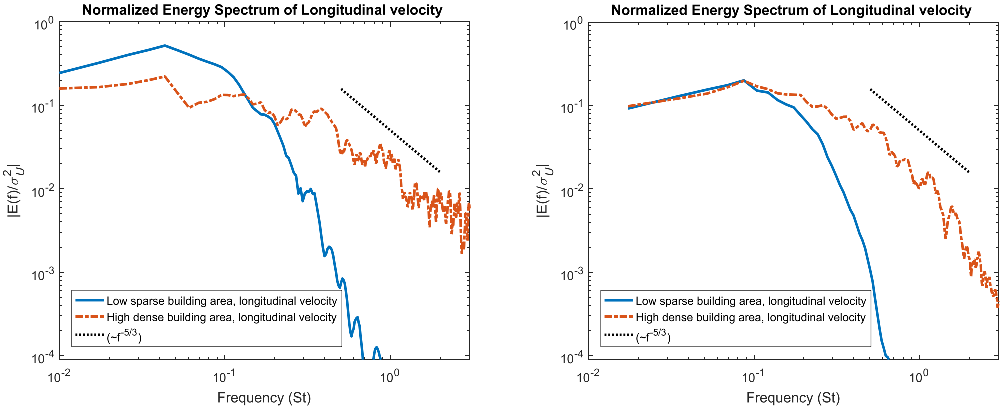


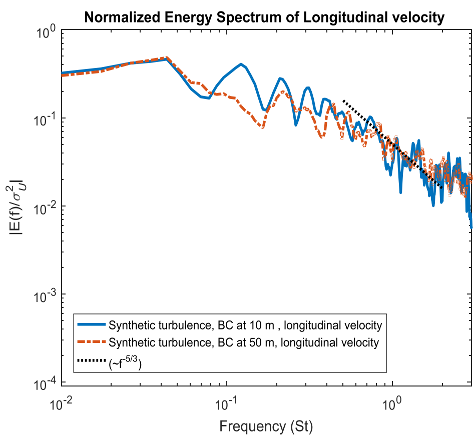
Figure 2. Normalized energy spectrum for longitudinal velocity at the probe positions in the 'low sparse building area' and in the 'high dense building area', calculated *without* synthetic BC using the Smagorinsky model (left) and the SIGMA model (right).

In Figure 2 it is shown that at the location ´low sparse building area´ a turbulent boundary layer is not developed but at the ´high dense building area´ the normalized spectrum show an energy drop that follows the 5/3-law which indicates a well resolved LES. If a synthetic turbulence is used for the inlet boundary conditions, (see Figure 3 left pane) a turbulent field is present at the ´low sparse building area´, see Figure 3 right pane. The energy spectrum at the ´high dense building area´ is very little affected, possibly a larger part of the turbulent energy is located at higher frequency.

Measurements of turbulence during JU2003 here considered were performed at two towers corresponding to low and high building areas. Tower positions and data can be found in Garvey et al. (2009). In Table 1 the TKE values from the Towers and the models are found.

Dispersion

Figure 4 shows that the predicted mean of the normalized concentration C/Q s/m^3 by the Smagorinsky and SIGMA model are quite similar. The noted difference is that the SIGMA model shows a larger high-concentration area closer to the source. In agreement with the observation reported in Hanna et al. (2011), it is also found that the initial plume is mostly transported north along Broadway, with little upwind dispersion. In addition, for both SGS-models, the mean concentration exhibits almost no dispersion westerly along Main and a moderate spread easterly along Main, which seems to quantitatively agree with reported observations by Hanna et al. (2011) of the real plume.
However, simulations without synthetic BC exhibit a somewhat higher spread easterly than do the simulations with synthetic BC, where the dispersion tends more to the north.



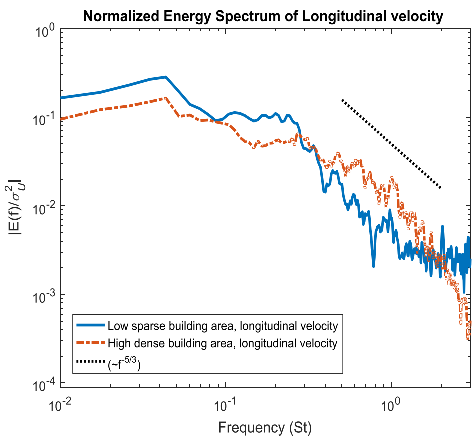


Figure 3. In the Left Pane the effect of the synthetic boundary condition is shown by the graph of the normalized energy spectrum of longitudinal velocity at the probe position next to the inlet boundary at two heights, 10 m and 50 m. In the Right Pane) it is seen that the turbulence is convected into the domain from the inlet boundary and induce a developed turbulent field. At higher frequencies dissipation is lacking which may be attributed to a coarser grid at the ´low sparse building area´ and also at the inlet boundary..

Table 1. The levels of measured TKE during JU2003 and simulated levels of TKE

LES-SGS-model	**TKE @ low sparse building area, m^2/s^2**	**TKE @ high dense building area, m^2/s^2**
Tower 1	>1,<3.2	-
Tower 2	-	>1,<3.6
Smagorinsky	0.01	1.73
SIGMA static BC	0.08	1.77
SIGMA synthetic BC	0.41	2.10

For both SGS-models the maximum concentration is one order of magnitude higher than the mean concentration up to approximately 150 m in the flow direction. In the maximum plots, it is also seen that the SIGMA model tends to spread more along Broadway, while the Smagorinsky tends to spread a bit more easterly.

CONCLUSIONS

Considering the 'high dense building area' the tested SGS-models are reasonably similar regarding the energy spectrum and dispersion. Therefore, the SGS-models could be useful, even without synthetic BC if the turbulence is mainly determined by the buildings and their configuration which is the case in the 'high dense building area', thus creating an urban boundary layer.

A large difference exists between the 'low sparse building area' and the 'high dense building area'. In the 'low sparse building area', it is essential to invoke synthetic BC to achieve a reasonable TKE level and mean wind profile that are representing the up-wind atmospheric properties. Within the predicted flow-path, tested modelling approaches produce reasonably similar predictions of maximum values, which in turn are reasonably similar to the experimental data. Thus, although spatiotemporal fluctuations obviously cannot be predicted in a directly useful way at specific points, there seems to be a strong possibility to use predicted maximum concentration values to render safer predictions, which could be particularly useful for casualty estimation in cases of a release of a hazardous gas in a city.

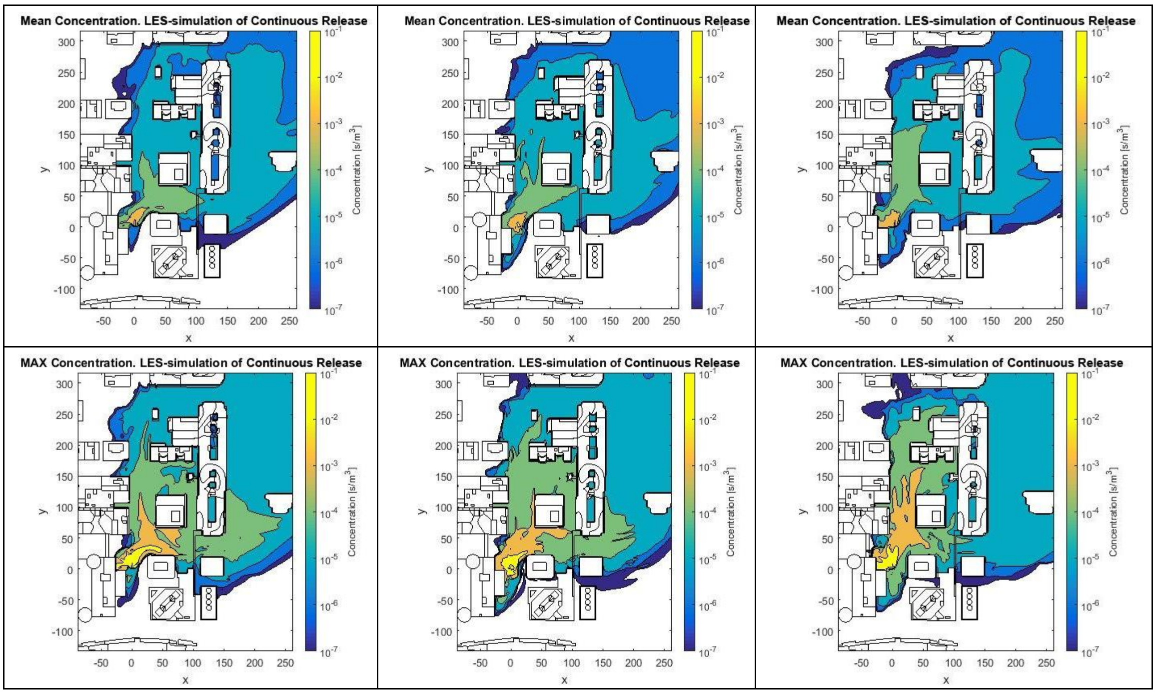


Figure 4. Contour plots of the predicted normalized concentration C/Q at 1.5 m height for a continuous release in IOP2 using the Smagorinsky model (left column) with static BC, the SIGMA model (middle column) with static BC, and the SIGMA model (right column) with synthetic BC. In the upper row, the mean of the concentration C/Q is shown, and in the lower row the maximum concentration C/Q is shown. The calculations of mean values and max values are performed from 115 s after the release until 360 s after the release, i.e., during a period of 245 s.

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