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MODITIC - LARGE EDDY SIMULATIONS OF DISPERSION OF NEUTRAL AND NON-NEUTRAL SCALAR FIELDS IN COMPLEX URBAN-LIKE GEOMETRIES

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Abstract: Release and dispersion of a neutrally buoyant and a dense gas is modelled using the LES approach in two urban-like geometries; an array of four cubes and a part of Paris. The description of the dense gas includes a variable density formulation and a Boussinesq approach, both of which are able to satisfactory predict the dense gas dispersion. Velocity- and concentration fields are compared to measurements from wind tunnel experiments and show overall good agreement. It is shown that the methodology used in the MODITIC project is well suited in order to model both dense and neutral gas dispersion in urban environments.

Key words: *MODITIC, Large Eddy Simulations, dispersion modelling, dense gas, neutral gas, urban environment*

INTRODUCTION

Release and aerial dispersion of toxic industrial chemicals (TIC) may threaten the lives and health of an urban population. In order to estimate the consequences and to identify most effective countermeasures to limit the impact, responsible authorities need to have reliable predictions of the spatial distributions as well as the time variations of the TIC concentrations. When considering non-neutral TIC, i.e., a denser-than-air or a lighter-than-air gas, the dispersion process poses sever challenges especially in complex urban environments and is an important area of research.

The transport and dispersion of pollutants in the atmosphere are governed by the conservation laws of mass, momentum, and energy. Non-neutral gases will predominantly be transported with the wind field, but the transport may also be significantly affected by e.g. the density differences, heat exchange, and gravitational force. The density difference may severely alter the turbulence field due to the resulting stably or unstably stratified background. The stratification primarily modifies the vertical mixing process of the plume, and therefore also the overall transport process. A neutral gas, i.e. a gas with the same density as air, on the other hand will be transported with the wind field without affecting its dynamics. In both cases it is the wind field that is the most important dynamical process, and in order to model the dispersion successfully, it is crucial to accurately model the wind field.

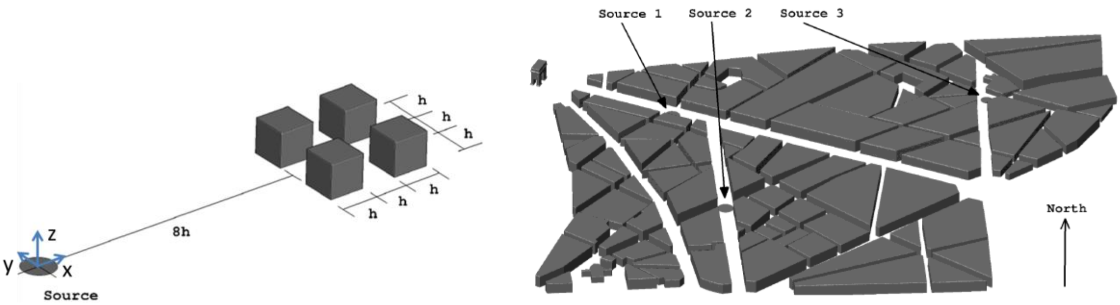
In the past two decades Computational Fluid Dynamics (CFD) has become a more popular tool for modelling dispersion. There exists a variety of different CFD models but the Large Eddy Simulation methodology seems to be most suitable for dispersion modelling in urban areas (Lateb et al. 2016). LES resolves the inherent unsteadiness of the large scale turbulence irrespectively of the nature of the averaged flow field. Previous studies using the LES approach for modelling the dispersion of neutral gases in urban areas have shown good results (cf. e.g. Boppana et al. 2010, Fossum et al. 2012, Liu et al. 2011).

This paper describes the work conducted using the LES approach to simulate release and dispersion of neutral and dense gas in urban-like geometries. The configurations consist of an array of four cubes and an actual urban area comprising a part of Paris. Three different solvers have been used (FDS, CDP and OpenFOAM) and the description of the dense gas includes both the variable density method and the

Boussinesq approach on incompressible flow. The purpose of the study is to improve the methodology for high fidelity dispersion models and validate the results to wind tunnel data.

SCENARIO DESCRIPTION

The transport and dispersion of a neutrally buoyant and a dense gas have been studied using both a large wind tunnel and numerical models, for two different urban-like geometries. The first consists of four cubes, with height h=0.11 m, mounted on a flat plate which are to resemble an urban street canyon. The second case is an urban area of parts of Paris in scale 1:350, which in full scale correspond to approximately 2 km^2. In the latter case, two different source locations are considered (source 1 and 2) whereas only one is considered in the former (see Figure 1).



(a) Case 1: Array of four cubes. *(b) Case 2: Paris.*

Figure 1. Schematics of the two configurations (a) four cubes and (b) Paris.

Flow parameters defining the incoming flow field and the emission can be found in Table 1. The dense gas used in this study is CO_2, which is approximately 1.5 times heavier than air.

Table 1. Parameters describing the incoming wind field and source characteristics.

Parameter	**Emission rate Q (dm^3/min)**	**Source diameter d (m)**	**Reference velocity U_{ref} (m/s)**	**Boundary layer height H (m)**	**Friction velocity U^*/U_{ref}**
Value	50	0.1	1	1	0.055

MATHEMATICAL MODELLING

In LES, the filtered Navier-Stokes equations are solved numerically and the small scale turbulence is modelled using a sub-grid scale model. There exist a wide range of different sub-grid models and in this study both the dynamic Smagorinsky model (DS) and the localized dynamic kinetic energy model (LDKM) is used. The dynamic process governing the transport of a scalar field is described by a Eularian convection – diffusion equation. The effect of dense gas is accounted for using either a Boussinesq approach, assuming small density variations, or with a variable density formulation. In Table 2, simulation parameters for the different solvers used are stated.

Table 2. Simulation parameters for the different solvers used by the partners in MODITIC.

Solver	**Dense gas description**	**Sub-grid model**	**Wall functions**	**Inflow conditions**
CDP	Variable density	DS	No	Roughness elements
FDS	Variable density	DS	Yes	Synthetic turbulence
OpenFOAM	Boussinesq	LDKM	No	Roughness elements

Two methods for generating the inflow boundary layer from the wind tunnel are adopted; synthetic turbulence and roughness elements. Both methods are described in detail in Osnes et al. (2016).

RESULTS AND DISCUSSION

In the following evaluation, computed flow quantities and concentrations are compared to experimental wind tunnel measurements.

Case 1: Array of four cubes

Figure 2 displays the vertical variation of the mean streamwise velocity component across the boundary layer for neutral and dense gas release at a position located in between the cubes (x,y)=(9.5h,0) (cf. Figure 1a) using the CDP solver. Similar profiles are observed with the FDS solver. Comparison with the experimental data shows very good agreement and we are able to predict the effect of the dense gas release on the wind field.

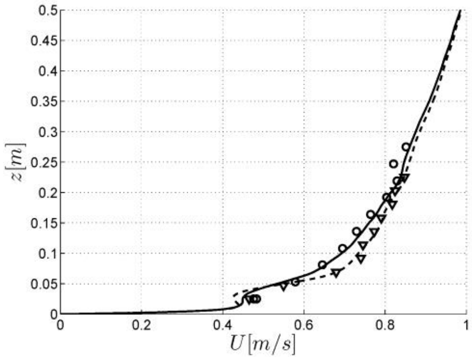
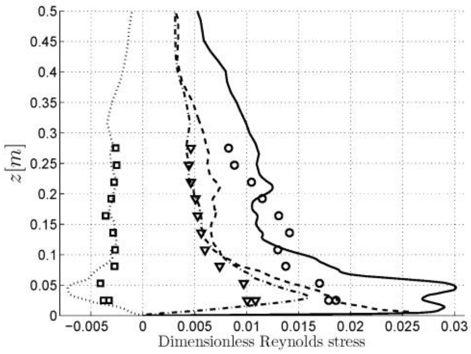
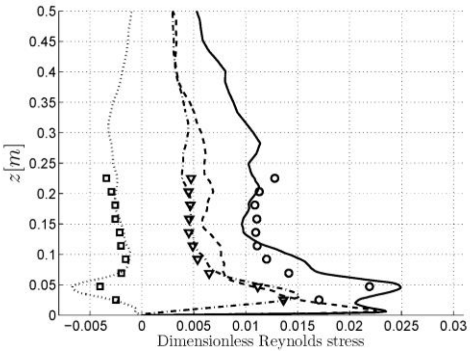


Figure 2. Vertical profiles of mean streamwise velocity for neutral and dense gas release at (x,y)=(9.5h,0). Symbols denote experimental measures (neutral ○, dense ▽) and lines numerical results (neutral ——, dense ---) using the CDP solver.

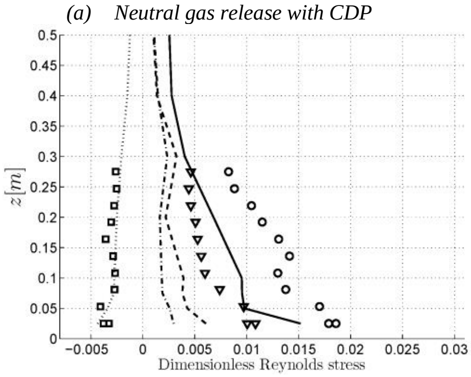
Figure 3 shows the vertical distribution of the dimensionless Reynolds stresses taken in the same position as in Figure 2. The dominating Reynolds stresses are predicted with good results for both the neutrally buoyant (Figure 3a,c) and the dense gas *(*Figure 3b,d). FDS gives a slight underprediction of the stresses which is most likely due to the synthetic turbulence at the inflow and the grid resolution. The release of dense gas seems to affect the level of turbulence kinetic energy.



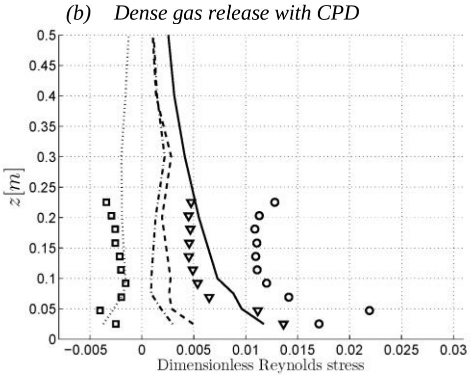
(a) Neutral gas release with CDP



(b) Dense gas release with CPD



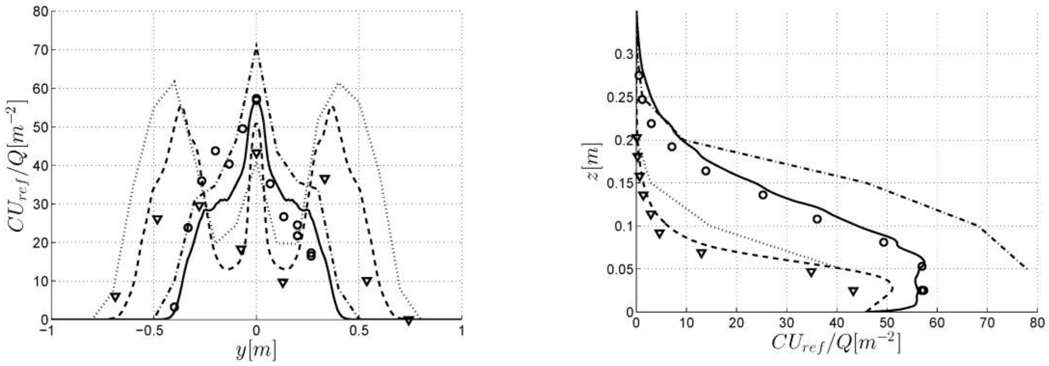
(c) Neutral gas release with FDS



(d) Dense gas release with FDS

Figure 3. Vertical variation of Reynolds stresses at (x,y)=(9.5h,0). Symbols illustrate experimental measures and lines show numerical result. $\langle u'u' \rangle$ (○, ——), $\langle v'v' \rangle$ (---), $\langle w'w' \rangle$ (▽, -.-) and $\langle u'w' \rangle$ (□, ······).

In Figure 4 the mean concentrations are compared to experimental results. The height and width of the dispersed plumes are predicted with good agreement. The FDS solver yields slightly higher concentrations which could be due to the reduced mixing stemming from lower turbulence kinetic energy. There is a very different dispersion pattern between the dense and the neutral gas. The dense gas forms a wider and shallower plume which is mostly deflected around the cubes, whereas the neutral gas passes through them.

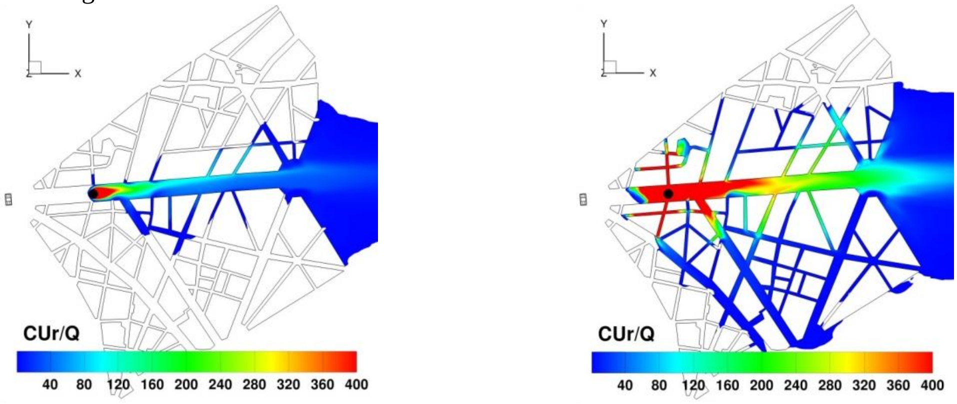


(a) Lateral concentration profile at (x,z)=(9.5h,0.25h) *(b) Vertical concentration profile at (x,y)=(9.5h,0)*

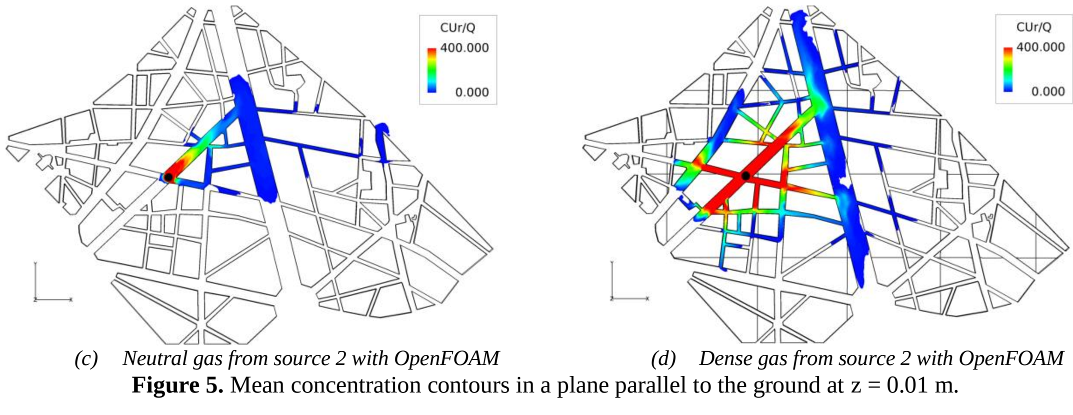
Figure 4. Mean concentrations for neutral (Experiment ○, CDP ──, FDS -.-) and dense gas (Experiment ▽, CDP ---, FDS ·····).

Case 2: Paris

The difference between the dispersion of a neutrally buoyant and dense gas close to the ground in Paris are visible in Figure 5.



(a) Neutral gas from source 1 with CPD *(b) Dense gas from source 1 with CDP*



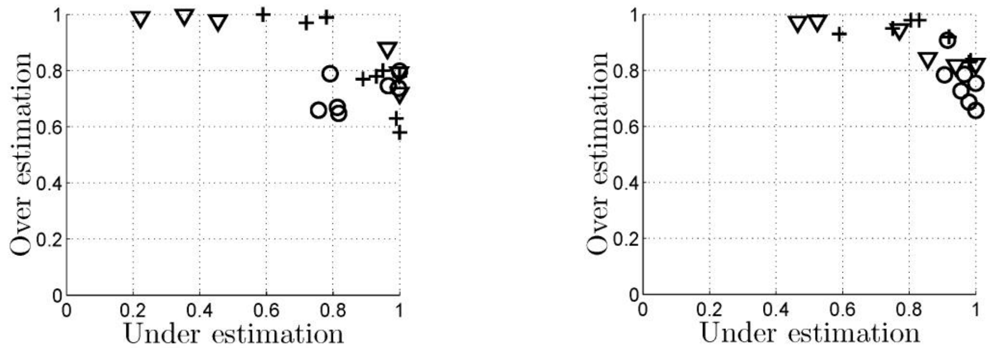
(c) Neutral gas from source 2 with OpenFOAM *(d) Dense gas from source 2 with OpenFOAM*

Figure 5. Mean concentration contours in a plane parallel to the ground at z = 0.01 m.

The dense gas has a larger spanwise and shallower plume spread, with higher concentrations close to the ground, compared to the neutral gas. Interesting is the upstream transport for the dense gas (see Figures

5b,d). The interaction between the dense gas release and the wind field in the vicinity of the source results in a horse-shoe type vortex that transports the gas upstream. Similar results for source 1 (cf. Figure 5a,b) are observed for the FDS solver. Even if different source locations and dense gas models are used, similar dispersion effects are observed. Hence, the variable density and the Boussinesq approximation, assuming small density variations, seem to capture the dispersion pattern similarly.

In Figure 6, lateral and vertical measurements are compared to experiments using a method called Measure of efficiency (MOE) (Warner et al. 2001). A value of (1,1) corresponds to a perfect agreement with measurements, while a value of (1,<1) indicate that the model overpredicts the concentration at all positions. Similarly, if the MOE gives a value of (<1,1), the model underpredicts the concentration field.



(a) Neutral gas *(b) Dense gas*

Figure 6. Measure Of Efficiency. CDP (○, source 1), FSD (▽, source 1) and OpenFOAM (+, source 2).

The MOE from the dense gas simulations gives slightly better results, especially when using the FSD and OpenFOAM solvers. The CDP code produces fairly consistent results for both neutral and dense gas releases which is very encouraging. It should be noted that most of the dense gas stays within the street network where the wind field is less sensitive for deviations from the experimental incoming boundary layer compared to the neutrally buoyant gas that mostly spreads above roof height.

CONCLUSION

In this study, dispersion of neutral and dense gas in urban-like geometries has been modelled using LES. The results are compared to wind tunnel experiments and both the velocity- and concentration fields show good agreement. Due to the coupling with the wind field, dense gas is dispersed differently than the neutral gas, with higher concentrations close to the ground, upwind spread, and a wider plume. The neutrally buoyant gas is to a higher degree transported above the building-like structures, where the wind field is more affected by the atmospheric boundary layer. In order to accurately predict the dispersion above building structures it is crucial to have appropriate inflow conditions. Both the variable density method and the Boussinesq approach imbedded within the framework of LES give acceptable results for urban dispersion.

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