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A CFD MODELING APPROACH FOR A CONTAMINANT RELEASED IN A CITY

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Abstract: In the context of industrial risk management, occurring at urban scales, decision-making processes remain subject to various sources of uncertainty and required accurate and realistic models to simulate atmospheric pollutant diffusion both in forward and inverse modelling. In the frame of this work, the three-dimensional (3-D) computational fluid dynamic (CFD) model OpenFOAM adapted to the dispersion of toxic and hazardous gases around buildings has been evaluated. In this study, OpenFOAM model is utilized to evaluate the Mock Urban Setting Test (MUST) field tracer experiment that provide a simplified urban-like area. A statistical analysis was performed to compare the concentrations from CFD model simulations with the experimental measurements. A detailed analysis with statistical measures shows that the performance of OpenFOAM model against observations is well within the acceptable bounds of statistical measures for air quality applications. The CFD model predicts 83% of the total concentrations within a factor of two and shows the over-prediction tendency at the receptors near to the source but under-prediction at far away from the source.

Keywords: *CFD modeling, MUST experiment, OpenFOAM, Urban dispersion modelling.*

INTRODUCTION

Air quality assessment in complex urban terrain with new and existing techniques is imperative to provide the information needed to estimate the population exposure to hazardous airborne matter and to assist regulators, urban planners or emergency authorities to outline the evacuation plans in a case of the natural disasters, accidental or deliberated release. In urban sites, dispersion of toxic gases surrounding the buildings are often predicted with Computational Fluid Dynamic (CFD) codes. A CFD model solves the Navier-Stokes fluid dynamics equations using a small grid size (of the order 1 m or even 12 less) (Hanna et al., 2004) over the complex terrains. Many CFD codes were successfully evaluated against experimental data for various types of releases in diverse geometric environments and atmospheric conditions (Rakai et al., 2014; Labovsky and Jelemensky, 2010; Gromke and Blocken, 2015; Kumar et al., 2015; Efthimiou et al., 2015; etc.). However, to obtain the reliable results for emergency preparedness and air quality analysis, the CFD models are required to be set up, tested, and evaluated correctly with the experimental observations in different geometric environments and atmospheric conditions (Tominaga and Stathopoulos, 2013). Complexities in flow fields and pollutant transport and dispersion in urban region make difficult to assess the contaminant plume concentrations due to local topography, terrain conditions, buildings and other geometrical structures. This study concerns the evaluation of a CFD model OpenFOAM against the Mock Urban Setting Test (MUST) field tracer experiment environments. In order to evaluate the CFD simulations of urban flows and pollutant dispersion, the completeness and the reliability of the experimental data is a necessity. This study utilizes one trial of the MUST field experiment in order to demonstrate the OpenFOAM model's capabilities to simulate the flow and dispersion patterns in the near field but also at larger distances.

MOCK URBAN SETTING TEST (MUST) FIELD EXPERIMENT

In the present study, we have used the observations taken from the MUST field experiment conducted at the U.S. Army Dugway Proving Ground (DPG) Horizontal Grid test site (40°12.606' N, -113°10.635' W) on 6-27 September 2001 (Biltoft, 2001). The test site was primarily flat with an averaged momentum roughness length of 0.045 ± 0.0005 m, and the zero plane displacement height of 0.37 ± 0.09 m (Yee and Biltoft, 2004). The MUST experiment represent an urban roughness geometry by placing 120 shipping containers ordinary arranged in a large array of building-like obstacles. These containers (12.2 m × 2.42 m × 2.54 m) were placed in a regular formation of 10 rows and 12 columns forming an approximately 200 m × 200 m array. Thus the terrain was considered as an idealized urban-like terrain in the computation. The MUST experiments was conducted mostly in neutral and stable atmospheric conditions. A detailed description of the meteorological and tracer observations are given in Biltoft (2001) and Yee and Biltoft (2004) that includes an extensive meteorological observations within and around the test site to characterize flow fields, turbulence, temperature and momentum gradients and fluxes, and atmospheric stability (Biltoft, 2001). One case #2681829 (Date: 25-09-2001, Time: 1830 MDT) is selected in the present study for the dispersion of a Propylene (C_3H_6) pollutant. In this selected case, 225 l min^{-1} Propylene was continuously released in the atmosphere for 15 min from a 1.8 m source height and measured at 48 receptors points (both horizontal and vertical cross-sections of the dispersing plume) downwind from the source (Figure 1). The concentration measurements were recorded at the height of 1.6 m (at 40 receptor points, in red color in the Figure 1) and 1, 2, 4, 6, 8, 10, 12, and 16 m (at 8 receptors in vertical direction on a single point in the domain, in green color in the Figure 1) above the ground level at the frequency response of 50 Hz. The mean wind speed and direction at South tower upstream the array at 4 m height above the ground surface were 7.93 ms^{-1}, and -41° respectively (Yee and Biltoft, 2004). The atmospheric stability was neutral (Obukhov length LMO = 28000 m) during this experimental case (Table 1). By following Yee and Biltoft (2004), 200-s quasi-steady periods within each 15-min plume dispersion experiment was extracted from the selected trial to remove the non-stationary from the data.

Table 1: Characteristics of the test case #2681829

U (m s^{-1})	α (deg)	σ_θ (deg)	k (m^2 s^{-2})	Q (L min^{-1})	z_s (m)	u^* (m s^{-1})	L (m)	ε (m^2 s^{-3})
7.93	-41	9.5	1.46	225	1.8	1.1	28000	0.8

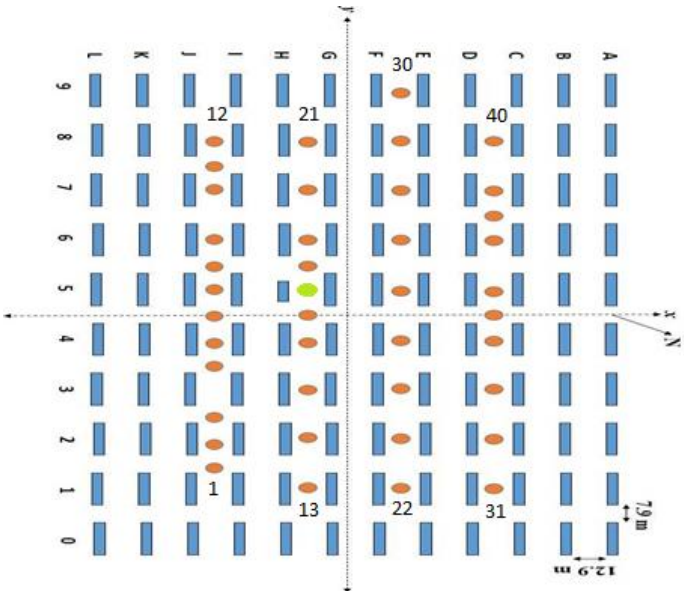


Figure 1: Representation of the MUST experiment with the location of measurement sensors

MODEL AND METHODS

In OpenFOAM, the equation of momentum, mass transfer and the turbulence model (Reynolds Average Navier Stokes (RANS) equation) for homogeneous multiphase flow are supposed to be solved using the finite volume method. Generating mesh using snappyHexMesh tool was used for the geometry. Using embedded meshing techniques, cells are concentrated around each container (Figure 2) in order to capture the detailed shear and entrainment effects at the edge of the gas column. Maximum distance of meshes near the initial plume is 0.5 m. Computational grids consist of 0.83 million cells. The convergence criterion was the residual of root mean square that was considered to be equal to or less than 10^{-4}. As mentioned earlier, C_3H_6 was used in the MUST experiment. Therefore this gas is considered in addition to air in the domain. The experiments were conducted at a neutral atmospheric condition and a standard k-ε model is used to simulate the turbulence processes. OpenFOAM was modified to estimate the turbulent kinetic energy and dissipation rate based on input Pasquill stability class or input of Monin-Obukhov length L. For the calculations of transport and dispersion of C_3H_6, the boundary conditions are usually either (i) no slip solid surfaces, (ii) wind inflow (or outflow), or (iii) a passive outflow condition at ambient pressure.

NUMERICAL SOLUTION AND DISCUSSION OF THE RESULTS

Figures 3a and 3b represents respectively the 2-D and 3-D contours plot of the steady CFD simulated tracer concentrations at ground level within the site. One can see that the plume disperses mostly in the direction of the mean wind. For a point to point evaluation of the model with observations, Chang and Hanna (2004) suggested to replace all those concentration values which are below detection limit of the samplers to that detection limit. The sampling calibration range of the detectors used in MUST experiment was 0.04-1000 ppmv (Biltoft, 2001).

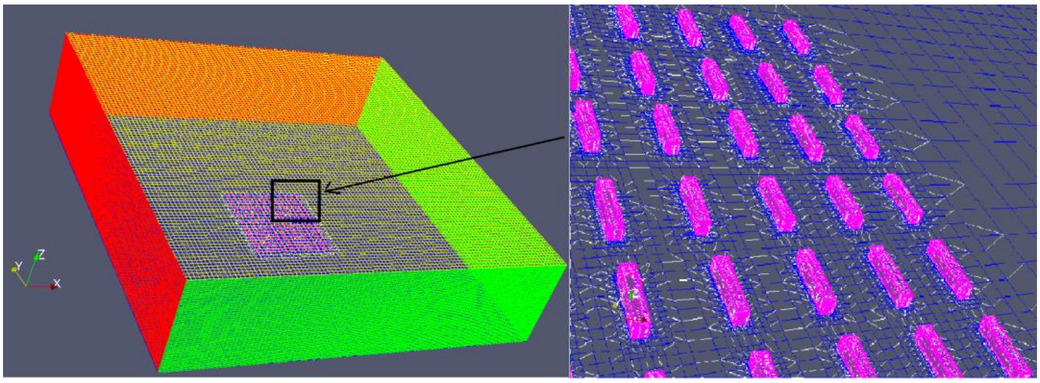
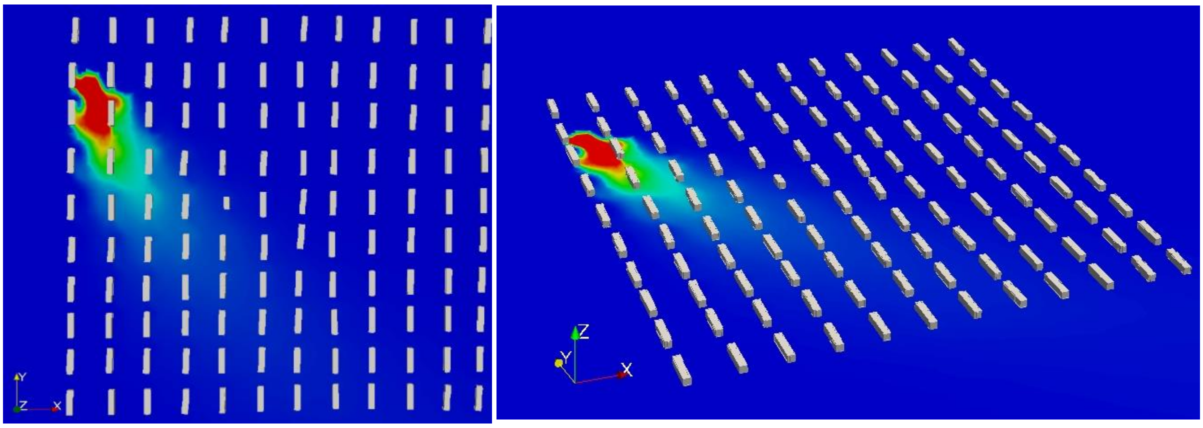


Figure 2: Site features and generating mesh using snappyHexMesh in OpenFOAM

By following Donnelly et al. (2009), the lower concentration value from the detection limit in any pair from all the pairs of model and observations is set to the detection limit 0.04 ppmv. If both concentrations in one of the pair are below the detection limit, both have been set to zero and removed from the dataset.



(a) 2D (b) 3D

Figure 3: Ground level concentration contours (in ppmv) computed from steady CFD solution for the case #2681829 of MUST Experiment (α=–41°) (a) 2D view, (b) 3D view. Here, the maximum concentration of C_3H_6 is 5 ppmv (red color on the isopleths).

Experimental measurements indicate in the Figure 4 that detectors n°8 and n°9 (from Figure 1) are the most exposed to the plume (at least 3 ppmv). Four secondary peaks of concentrations are also observed, but their intensity is at least two times lower (between 1 and 1.7 ppmv). It is clear that the OpenFOAM model underestimate the concentrations obtained experimentally. The biggest disagreement is found in the last 8 sensors on the central mast at different heights. It follows that the gas plume does not appear to rise in sea level, and is conditioned by the surface roughness (here the containers). This is one of the characteristics of the flows in a neutral atmosphere. Indeed, the performance of the model is also analysed using the standard statistical performance measures (Chang and Hanna, 2004) such as Normalized Mean Square Error (NMSE), Fractional Bias (FB), Correlation coefficient (COR), Fractional Variance (FS), and Factor of Two (FA2). These measures characterize the agreement between model prediction and observations. The NMSE emphasizes the scattering in a sample and FB indicates an overall over or under-prediction from the observations. A prefect model would have the following idealized values: NMSE = FB = FS = 0 and COR = FA2 = 1 (Chang and Hanna, 2004). The predicted and observed concentrations at all receptors are presented in forms of the scatter plots (Figure 5a) and the Q-Q plots (Figure 5b). In the scatter plots (Figure 5a), it is observed that the simulated concentrations by the CFD model have relatively good agreement with the observations. The simulated higher concentrations at the receptors near to the source are close to one-to-one line; however, comparably more scatter is observed for lower concentrations at far away from the source. This trend of the predicted concentrations is more visible in Q-Q plot in Figure 5b. This Q-Q diagram shows a comparison of the concentration distributions of simulated and observed concentrations. The computed statistical indices are given in Table 2. The computed statistical indices for CFD simulation show that the OpenFOAM is preforming good with the observations. The model predicts 83.3% of points within a factor of two. The FB shows that the extent of under- or over-prediction the simulated concentrations from the observations. It shows that similar degree of a slightly under-prediction (FB = 0.11) was observed. Good one-to-one correlations can be observed by the higher values of correlation coefficient (COR=0.87). The values of MG (=0.97) and VG (=1.33) show a small scatter and it is also visible from the scatter and Q-Q plots in Figures 5a-5b. Hence, the statistical evaluation results show an overall good performance of the CFD model in such complex environment. The CFD model OpenFOAM used in this study is well suited for the air pollution and emergency planning in urban area.

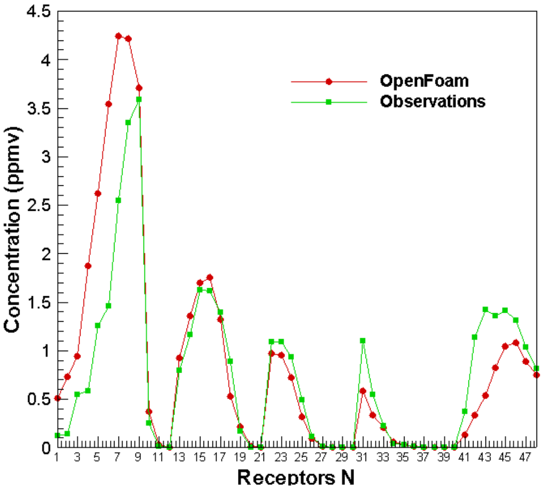
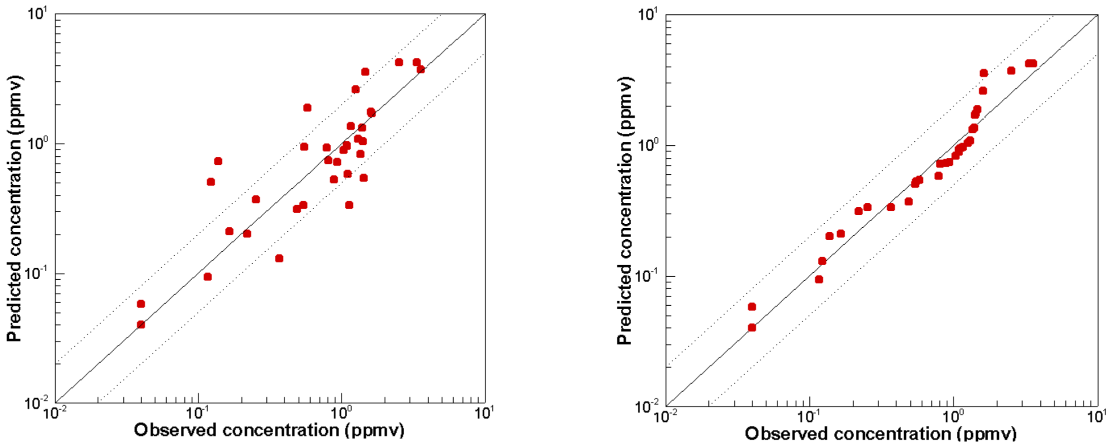


Figure 4: C_3H_6 concentration (in ppmv) at each sensor



(a) (b)

Figure 5: (a) Scatter and (b) quantile-quantile (Q-Q) plots between the predicted and observed average concentrations. The middle solid line is one-to-one line between observed and simulated concentrations whereas the dotted lines correspond to factor of two.

Table 2: Statistical indicators of model quality

<Co>	<Cp>	NMSE	MAE	RMSE	COR	FB	FS	FAC2	MB	VAR	INDEX	MG	VG
0.76	0.85	0.47	0.30	0.55	0.87	0.11	-0.54	83.3	0.09	0.55	0.91	0.97	1.33

CONCLUSIONS

This study presents the three-dimensional CFD simulations for near-field dispersion of pollutant near buildings. A CFD model OpenFOAM is evaluated with the concentrations measurements obtained from a trial of the MUST field experiment in an urban-like environment. The model is simulating well with the observations for the selected trial in a complex terrain and predicts ~83% concentrations within a factor of two. The modelled concentrations are slightly over-predicting with the observations and have relatively good correlation (COR =

0.87) between them. This first comparison shows an adequate agreement between the modelled values and the measured concentrations. Further, the model has been coupled in inverse mode, based on renormalization theory, for identifying a point source release in an urban like environment of MUST field experiment. The study is underway to highlight the detection feasibility of unknown releases in an urban-like environment with a use of more sophisticated model like OpenFOAM. The study will show the effectiveness of the renormalization inversion technique to estimate the source parameters in an urban area. Estimating the source height along with the other source parameters may further improve the retrieval results and it need to be verified with the available observations in other trials of the MUST field experiment.

REFERENCES

Biltoft, C. A., 2001: Customer Report for Mock Urban Setting Test, DPG Document No. WDTCFR- 01-121, West Desert Test Center, U.S. Army Dugway Proving Ground, Dugway, Utah, 58 pp.

Chang, J. C. and S. R. Hanna, 2004: Air quality model performance evaluation. *Meteorol. Atmos. Phys.*, 87, 167-196.

Donnelly, R. P., T. J. Lyons and T. Flassak, 2009. Evaluation of results of a numerical simulation of dispersion in an idealized urban area for emergency response modelling. *Atmospheric Environment* 43, 4416-4423.

Efthimiou, G. C., Berbekar, E., Harms, F., Bartzis, J. G., Leitl, B., 2015. Prediction of high concentrations and concentration distribution of a continuous point source release in a semi-idealized urban canopy using CFD-RANS modeling. *Atmospheric Environment* 100, 48–56.

Gromke, C., Blocken, B., 2015. Influence of avenue-trees on air quality at the urban neighborhood scale. Part I: Quality assurance studies and turbulent Schmidt number analysis for RANS CFD simulations. Environmental Pollution 196, 214–223.

Hanna, S. R., Hansen, O. R., Dharmavaram, S., 2004. FLACS CFD air quality model performance evaluation with kit fox, must, prairie grass, and EMU observations. *Atmospheric Environment* 38 (28), 4675-4687.

Kumar, P., Feiz, A.-A., Ngae, P., Singh, S. K., Issartel, J.-P., 2015. CFD simulation of short-range plume dispersion from a point release in an urban like environment. *Atmospheric Environment* 122, 645-656.

Labovsky, J., Jelemensky, L., 2010. CFD simulations of ammonia dispersion using dynamic boundary conditions. Process Safety and Environmental Protection 88 (4), 243 – 252.

Rakai A., Berbekar E., Franke J., 2014. RANS Passive Scalar Transport Modelling in a Complex Urban Area–Effect of Source Location on the Results, *6th International Symposium on Computational Wind Engineering*, 116-117.

Tominaga, Y., Stathopoulos, T., 2013. CFD simulation of near-field pollutant dispersion in the urban environment: A review of current modeling techniques. *Atmospheric Environment* 79 (0), 716-730.

Yee, E. and C. A. Biltoft, 2004: Concentration fluctuation measurements in a plume dispersing through a regular array of obstacles. *Boundary-Layer Meteorol.*, 111, 363-415.