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APPLICATIONS OF A CFD MODEL FOR SHORT-RANGE POLLUTANT DISPERSION AND SOURCE RECONSTRUCTION IN AN URBAN ENVIRONMENT

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Abstract: Dispersion of air pollutants in an urban environment is a challenging problem due to the complexity in interaction of plume and flow field perturbed by the obstacles. The increasing threat of chemical, biological and radiological (CBR) attacks in urban areas has also resulted a significant interest in research on fast identification and detection of these toxic agents. In this study, a computational fluid dynamics (CFD) 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. Further, the model has been coupled in adjoint mode with a recently proposed inversion technique, based on renormalization theory, for identifying a point source release in an urban like environment of MUST field experiment. The study highlights the detection feasibility of unknown releases in an urban-like environment with a use of more sophisticated model.

Key words: *CFD modeling, Dispersion, Inverse problem, MUST field experiment, Renormalization theory.*

INTRODUCTION

Accurately simulation of the atmospheric pollutant dispersion and an estimation of the source parameters (location and strength) from the limited information by a finite set of the meteorological and concentration measurements in an urban area are crucial for emergency preparedness and mitigation process. The source retrieval problem is necessarily addressed by use of a dispersion model and effectiveness of the estimation is highly subjected to the performance of dispersion model. The intricacy of the source estimation in a complex terrain increases due to the uncertainty in the simulated wind flow that generally affect the plume dispersion in that region. The real flow field in an urban area is significantly influenced and perturbed by the obstacles/buildings in that region. Recent advancement in the numerical models like Reynolds Average Navier Stocks (RANS) equation, Large Eddy Simulation (LES), and Direct Numerical Simulation (DNS), etc. that accurately simulate the flow field in an urban area is a significant step towards the accuracy of plume dispersion and inversely for source retrieval. With advancements of the computational resources, these Computational Fluid Dynamics (CFD) models are increasingly being used to simulate the transport and dispersion of pollutants in an urban area (Donnelly et al., 2009). Various studies were performed for a point source estimation over the flat, uniform, and homogeneous terrain (Sharan et al., 2009, 2012; etc.) in various atmospheric stability conditions. However, only few studies were performed over a complex urban environment (Keats et al., 2007) where the estimation required the most in a case of emergency preparedness. In this study, a CFD model is used to evaluate in an urban-like environment of the Mock Urban Setting Test (MUST) field experiment. To identify the release source parameters in an urban area, a computationally method is described that utilizes an inversion technique based on renormalization theory (Issartel et al., 2007). The concentration and meteorological measurements from a continuous release of the MUST experiments is used for illustrating the renormalization technique in an urban area.

MOCK URBAN STETTING 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 forward dispersion of a pollutant and inversely for a point source retrieval in an urban-like environment. In this selected case, 225 l min^{-1} Propylene (C_3H_6) 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. The concentration measurements were recorded at the height of 1.6 m (at 40 receptor points) and 1, 2, 4, 6, 8, 10, 12, and 16 m (at 8 receptors in vertical direction on a single point in the domain) 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 L_{MO} = 28000 m) during this experimental case. 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.

MODEL AND METHODS

This study utilised a model Fluidyn-PANACHE® to compute the full-flow and dispersion of pollutants in the complex geometries. Fluidyn-PANACHE® is a 3-dimensional Computational Fluid Dynamics (CFD) diagnostic model for simulating atmospheric processes related to the pollution and hazard in complex geometric environment. PANACHE solves the Navier-Stokes governing air motion using 3-dimensional finite-volume techniques and includes a built-in automatic 3D mesh generator that can create the computational finite-volume mesh around obstacles and body-fitting the terrain undulations (Fluidyn-PANACHE®, 2010). The study domain for numerical simulations comprises outer and inner (nested) domains. Since the overall width and length of the obstacles array in MUST experiment were 193 m and 171 m (Yee and Biltoflt, 2004), the inner domain was considered 250 m × 225 m. To ensure a smoothly varying wind flow over the boundary, outer domain boundary was kept away from obstacles and thus, the size of the outer computational domain was considered 800 m × 800 m (approximately four times of the inner domain consisting the obstacles arrays). The heights of the inner and outer domains were taken as 100 m and 200 m respectively. The mesh can be structured (rectangular) or unstructured (triangular) in PANACHE. Clustering of mesh points in certain regions is also possible with nested domains. The mesh in this study is chosen to be unstructured for both outer and nested domains. The computational domain consist of total 559746 grid cells in the embedded mesh. Dispersion of gaseous pollutants is modelled by solving the standard Eulerian advection-diffusion equation governing the transport of species concentration. PANACHE has 3 turbulence models (k-diffusion, k-L, and k-ε) all of which are based on surface layer similarity theory. A k-ε 3D-prognostic turbulence model is used in this study. Residuals were used to check the convergence of the solution during simulation and in an ideal run, all the residuals was considered to be equal or less than 10^{-3}.

To retrieve the location and intensity of a continuous point source in the studied test-case of MUST field experiment, a technique based on the concept of the renormalization theory (Issartel et al., 2007; Sharan et al., 2009) is utilized in this study. This technique returns an emission estimate linear with respect to the finite number of concentrations measurements (Sharan et al., 2009). The renormalization theory required to compute the retroplumes as the adjoint functions of the concentration measurements at each receptor. PANACHE simulation for the meteorological field, along with the dispersion model is used to generate these retroplumes. The renormalization technique utilised these retroplumes to compute the weight functions corresponding to each concentration measurements at the receptors, and then these weight functions along with the concentration measurements identified the source parameters. In that case, the maximum value of the estimate coincides with the position of the source. A detailed step-by-step description of the renormalization theory for a continuous point source retrieval and various issues and limitations are given in Sharan et al. (2009).

RESULTS AND DISCUSSION

Figure 1 shows the isopleths of PANACHE's simulated dispersion plume at the ground surface in the computational domain. One can clearly 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). By following Donnelly et al. (2009) when any pair from all the pairs of model and observations, one of the concentration in that pair is below detection limit and other is greater than it, the lower concentration value from the detection limit 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. 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).

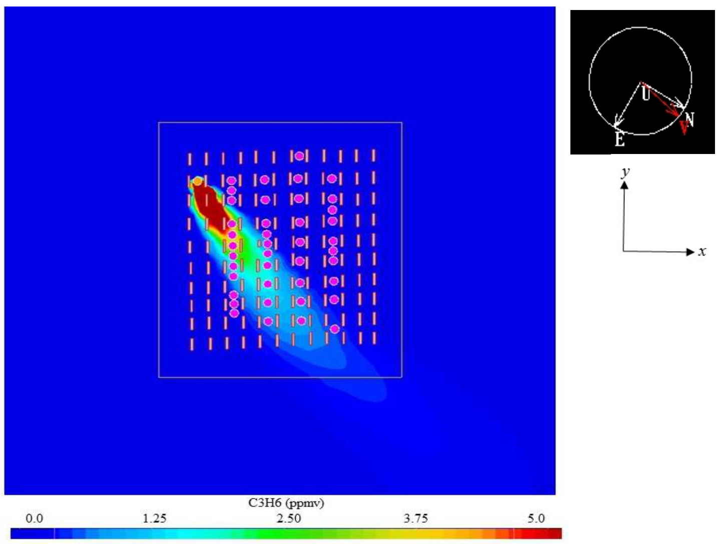

Figure 1. The isopleths of the model simulated ground level concentrations (in ppmv) of C_3H_6 for trial #2681829 (Date: 25-09-2001, Time: 1830 MDT) of the MUST field experiment. A yellow coloured filled circle is the location of the emitting point source and the pink spots representing the 48 receptors. The grid orientation and its geophysical direction from the North, and wind direction during the experiment is also visible from the coordinates axis and compass aligned with upper right corner.

Figure 2a shows a scatter diagram between the predicted and observed concentrations for the selected trial from MUST field experiment. It shows that satisfying agreement is found between tracer gas dispersion field measurements and the concentrations computed from the dispersion model. For an unpaired analysis, a Q-Q plot (Figure 2b) is drawn by arranging the both observed and predicted concentrations in increasing order of their magnitudes. This Q-Q plot reveals that the predicted concentrations are close to a one-to-one line. This fact is re-affirmed from the computed statistical measures. The values of the statistical measure NMSE, FB, FS, COR, are FA2 are found to be 0.14, 0.13, -0.37, 0.94, and 0.82 respectively. It shows that model predicts ~82% of the observations within a factor of two. The positive value of FB shows that model is slightly under-predicting with the observations. It also shows that model's concentrations has good correlation (COR = 0.94) with the observations. The overall statistical measures indicate that the simulated concentrations have good agreement with the observations.

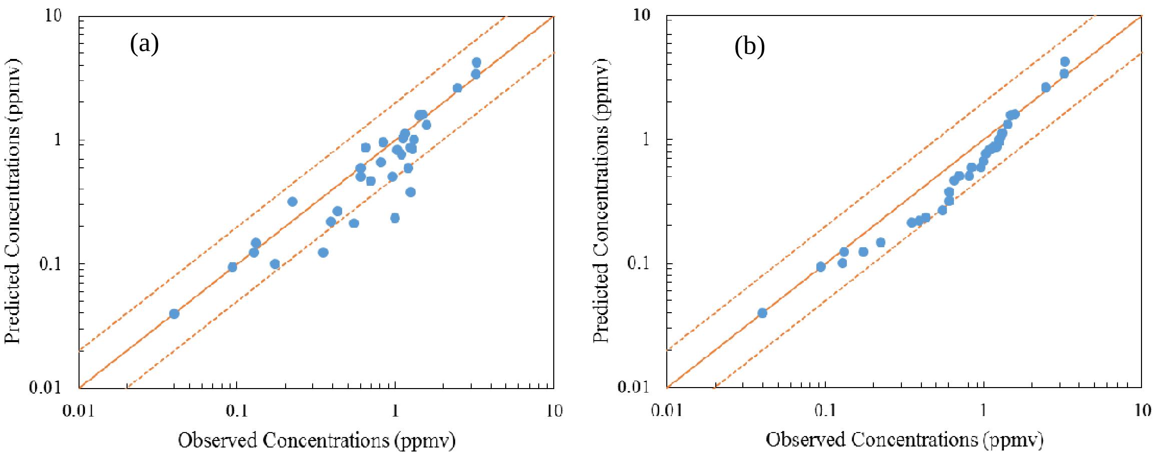

Figure 2. (a) Scatter diagram between observed and predicted concentrations for trial #2681829 of MUST field experiment, and (b) Q-Q plot between observed and predicted concentrations for the same case. Middle lines in both plots are one-to-one line and outer dotted lines are the lines with factor of two.

Concentrations measurements above the detection limit (i.e. 0.04 ppmv) were considered for source estimation. The concentrations measurements recorded at eight vertical level receptors located at a single point in the domain were also not considered for the computation of source estimation. In the studied trial of MUST experiment, the renormalization inversion technique used in this study retrieves the ground level source location to ~28 m Euclidean distance upwind from its true release location. The estimated source is located at a point (-99.12, 88.80), whereas the true release location was at (-77.46, 67.74) in the domain. The source strength was also estimated within a factor of ~1.5. The true source strength was 6.63×10^{-3} Kg/s; whereas 9.96×10^{-3} Kg/s Propylene was estimated from the inversion technique. The estimated source strength is over-predicting from the true source release. The results are further analysed from the contours of estimated source S(x) shown in Figure 3. The estimate S(x) provides a conditional distribution of emissions based on the information given by the available concentration measurements. Since source height is an important constituent affecting dispersion of the plume (Sharan et al., 2012), estimated source location and strength may further improve with retrieval of the source height in an urban like environment.

CONCLUSIONS

In this study, a CFD model Fluidyn-PANCHE® 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 ~82% concentrations within a factor of two. The modelled concentrations are slightly under-predicting with the observations and have good correlation (COR = 0.94) between them. The renormalization base inversion technique is also utilized to retrieve the location and strength of a continuous ground level point source in an urban-like area. With the real measurements from the selected trial in MUST field experiment, the source location is retrieved ~28 m distance upwind from its true release location. The estimated source strength is over-predicted by a factor of 1.5 of the true release rate. The study shows 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.

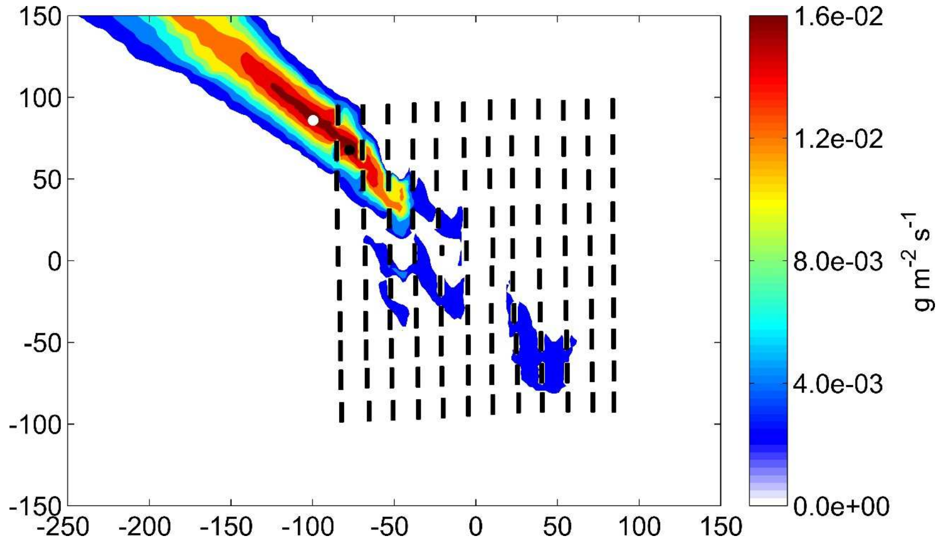

Figure 3. Contours of the estimate source S(x) (g m^{-2} s^{-1}) in the domain of trial #2681829 of MUST field experiment. The white coloured filled circle is the estimated source location and the black circle is the true location of source.

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