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CFD MODELLING OF ATMOSPHERIC DISPERSION USING NON-ISOTROPIC TURBULENCE MODEL: APPLICATION TO IDAHO FALLS EXPERIMENT IN LOW WIND STABLE CONDITIONS

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Abstract: The operational risk assessment and control during a pollutant release scenario requires, beforehand, an accurate simulation of the atmospheric dispersion phenomena. In this context, both the issues of low wind speed and that of stable atmospheric conditions remain a challenge to the numerical modeling of turbulent flows and dispersion at the local scale. In the frame of this work, a three-dimensional (3-D) computational fluid dynamic (CFD) model Code_Saturne®, adapted to the dispersion of hazardous gases in flat and complex terrains, has been evaluated. In this study, the atmospheric module of Code_Saturne® is used to evaluate the Idaho Falls field tracer experiment that provides a good example of release in low wind and stable atmospheric conditions. The CFD model performs acceptably by predicting almost all the concentration peaks. The analysis with statistical measures shows that the model predicts ~38% of the total concentrations within a factor of two and shows either under- or over-prediction tendencies that become more significant at the receptors far away from the source.

Key words: *CFD modelling, Idaho Falls field tracer experiment, low wind speed, stable conditions*

INTRODUCTION

Low-frequency meandering, characterized by important spatio-temporal variations in the direction of wind, occurs whenever the wind speed is below about 2 m/s. When these low wind conditions are coupled with strong atmospheric stability, longitudinal vortices in the horizontal axis, which are responsible for the meandering effect, become more important since the vertical motion is suppressed by buoyancy effects (Etling, 1990). From a point of view of the dispersion process, these conditions are the most penalizing since abnormally high concentration levels of pollutants can reside over time, at ground level up to several kilometers downwind from the source (Boyer et al., 1970). Several analytical dispersion models were used to deal with dispersion phenomena under low and variable wind conditions. One can cite the Gaussian puff/plume models (Luhar, 2011) (Sagendorf & Dickson, 1976), Lagrangian particle approach (Anfossi et al., 2006;Carvalho and De Vilhena, 2005; Oettl et al., 2001; Brusasca et al., 1992, etc). However, most of these models use different physical assumptions that make the modeling of the meandering effect far less realistic. For example, the classical widely-used Gaussian models are steady-state models that assume homogeneous wind-field during the sampling period, thus predicting very low ground-level concentration (Pandey & Sharan, 2019). CFD models, that solve Navier-Stokes equations using small grid sizes, have been proven to provide the efficient predictions of wind and dispersion fields regardless of geometric configuration, atmospheric conditions, and wind regimes. However, further research is still needed for a CFD solution involving a large variability in the wind configuration which can significantly affect the dispersion phenomena. The objective of this study is to evaluate a CFD model Code_Saturne® (EDF R&D) with the observations from the Idaho Falls tracer experiment (Sagendorf and Dickson, 1976). The reason for choosing this dataset is based mainly on the criterion that it contains sufficient instances of low wind speed and strong stable stability conditions. A single trial of the experiment is chosen to assess the ability of this code to simulate flow and dispersion patterns not only near the source but also at larger distances.

DESCRIPTION OF THE IDAHO FALLS FIELD EXPERIMENT

The Idaho Falls experiment (Sagendorf and Dickson, 1976), took place at the Idaho National Engineering Laboratory (INEL) in Southern-East Idaho (USA) in 1974. The experiment is conducted in a large and relatively flat terrain, under low wind speed and strong inversion conditions (Figure 1(a)). Wind measurements, including wind speed, wind direction, and standard deviationof the horizontal wind direction, were taken at six levels (2, 4, 8, 16, 32, and 61 m) on a 61 m heigh tower. The temperature profile was also measured at these heights and also at 1 m above the ground. A sulfur hexafluoride (SF_6) tracer was released at a height of 1.5 m above the ground. The concentrations were measured using samplers placed on three arcs of radius 100, 200, and 400 m from the source, at a height of 0.76 m above the ground. Because of wind direction variability, the sensors were placed at 6° intervals on each arc, thus forming a 360° sampling grid with 180 positions (Figure 1(b)). A total of eleven runs (run-4 to run-14) were carried out during the experimental campaign. Among the tests, there is a single test conducted under conditions of neutral stability and ten tests under conditions of stable stability. The duration of all runs was 1 hour, except for run-10 which lasted 49 min. For the present work, we select run-10 to simulate the flow of the wind and the dispersion of the passive tracer. This run is characterized by an extremely stable stratification. According to Carvalho and De Vilhena (2005), the Monin-Obukhov length (L) is equal to 5.93 m. The raw experimental dataset for the average wind speed (U) and wind direction (Θ), and the standard deviation (σ_Θ), is recorded at a reference height (z_r) of 4 m at every two minutes for a total duration of 49 min. The hourly-averaged values of these parameters are reported in Sagendorf and Dickson (1976). The aerodynamic roughness (z_0) length is estimated to 0.005 m (Brusasca et al., 1992).

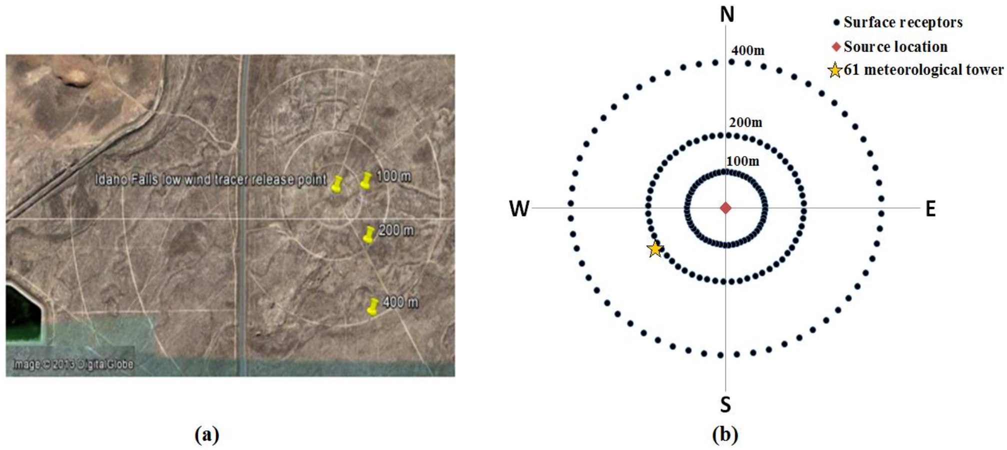

Figure 1. (a) Idaho Falls experiment site view (b) Schematic of Idaho Fall field with the location of the source and measuring sensors

NUMERICAL SETUP

In this section, we present the methodology of the numerical simulations of run-10 in Code _Saturne®. The three-dimensional and vertical grids of the computational domain are shown in Figure 2. For the continuous fluid phase, the turbulence model used is the second-order RANS Rij-ε model (Launder et al., 1975) which allows simulating the anisotropy of turbulence. Boundary conditions are imposed on the faces of the domain. An automatic inlet/outlet condition is set for the lateral boundaries of the domain since the dynamic profiles are varying in time. For inlet flow, a Dirichlet boundary condition is applied for velocity, temperature, and turbulent variables with analytical profiles based on the Monin-Obukhov similarity theory (MOST). The stability functions of Businger et al. (1971) are used to compute the average wind speed and temperature. The variables of turbulence, i.e. the kinetic energy and dissipation rate, are obtained using the parametrization of Dyer (1974). For outflow, a Neumann boundary condition is automatically imposed on the transported variables, except for the pressure. An inlet boundary condition is set for the top of the domain in order to maintain a continuous velocity profile. The ground is treated as a rough wall with a no-slip condition, and a roughness length of 0.005 m is imposed. The release of the passive tracer is modeled by a mass source term. A mass flow rate of 0.032 g/s is injected into a cell, close to the experimental release height (1.5 m). The concentration turbulent flux is modelled using the Generalized Gradient Diffusion Hypothesis (GGDH) algebraic model (Daly and Harlow, 1970). The simulation of the flow is carried out using an unsteady time algorithm. The continuous and dispersed phases are calculated simultaneously over a number of iterations in accordance with the duration of the variable meteorological file. Therefore, the performed simulations will count 29400 iterations for an average time step of about 0.1 s.

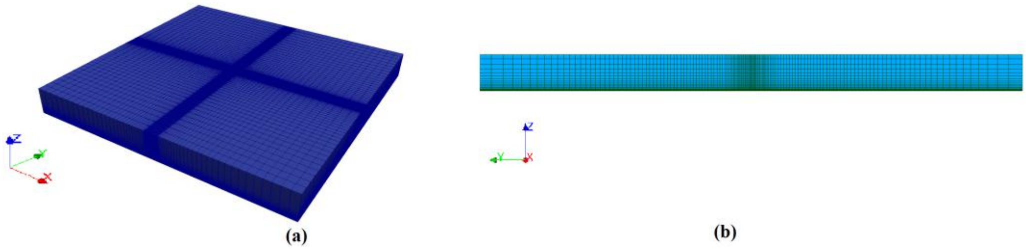

Figure 2. Mesh representation (L=W=900 m, H=60 m) for run-10 of Idaho Falls experiment (a) 3-dimensional view (400000 cells) (b) Vertical mesh. Close to the release point, the cells measure 0.72 m × 0.72 m × 1.2 m. The mesh is refined near the ground and the vertical resolution varies from 0.5 m to 7 m.

RESULTS AND DISCUSSION

The observed and predicted contour plots of ground-level concentration (CU/Q) are shown in Figure 3 (a) and (b), respectively. Both contours represent clearly the effect of plume meanders due to wind variability. The concentration distribution for both contour isolines varies from 3×10^{-6} m^{-2} to 0.001 m^{-2}. Qualitatively, the modeled contours are quite similar to the observed ones. However, the plume spread, which defines the sector width over which the SF_6 tracer is detected, is larger for the modeled contour than for the observed one. Table 1 shows the plume spread for both the observed and modeled contours, over the three arcs of measurement. The CFD model predicts concentration over seven additional receptors located at the arcs of 100 and 200 m, as well as over six additional receptors located at the arc of 400 m.

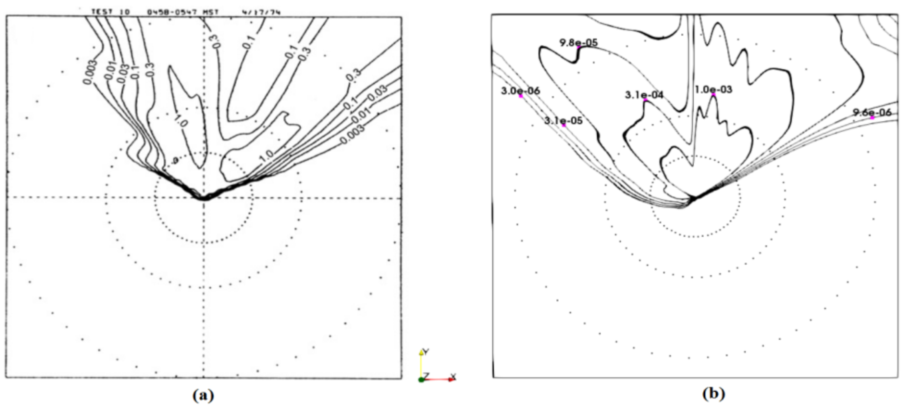

Figure 3. Contour plots of the ground-level concentration (m^{-2}) for run 10 showing (a) the observed concentration distribution (Sagendorf & Dickson, 1976); the values on the isolines must be multiplied by 10^{-3} (b) the modeled concentration distribution obtained from the CFD simulation.

Table 1. Comparison of the observed plume spread (degrees) to the modeled plume spread over the three arcs of receptors.

Arc radius (m)	100	200	400
Observed plume spread (degrees)	132	102	90
Modelled plume spread (degrees)	174	144	126

Figure 4(a), (b), and (c) show the observed and predicted concentration profiles on the three arcs of measurements, respectively. In accordance with the previous qualitative analysis, it is found that the concentration distribution is extended over a few receptors which makes the predicted profile wider than the observed profile, in the left part of the plot. We also noticed that the concentration peaks are almost predicted by the CFD model, despite the phase shift between the predicted profile and the observed one. Both under -and overestimating phases of the measured concentration alternate over the entire profile on the three arcs. This behavior is expected in a simulation involving a dispersion phenomenon under variable and low wind conditions. The performane of CFD model is evaluated using some statistical performance measures as well as using scatter and quantile-quantile (Q-Q) plots. In this step, all pairs of concentrations are eliminated, if the measured or predicted values or both are below the detection limit (10^{-7} m^{-2}). The scatter and (Q-Q) plots are shown in Figure 5. By examining the scatter plot, we noticed that a majority of the points are within the range of a factor of two or even very close to it. On the other hand, the CFD model tends to largely over- or under-estimate the measured concentration, especially far away from the source (400 m arc). The Q-Q plot generates a set of unpaired concentration values that are close to the one-to-one line. This shows that the distribution of the predicted concentrations is similar to the observed concentrations. The statistical performance measures are presented in Table 2. A model is considered perfect if: RMB-TT=NMSE = FB = FS = 0 and COR = FAC2 = IOA = VG = 1 (Chang and Hanna, 2004). The CFD model predicts 37.5% of points within a factor of two. The negative value of FB (-0.24) indicates a slightly overall over-prediction from the observations. The values of MG (=0.88) and VG (=11.1) show a large scatter, which is also visible from the scatter and Q-Q plots.

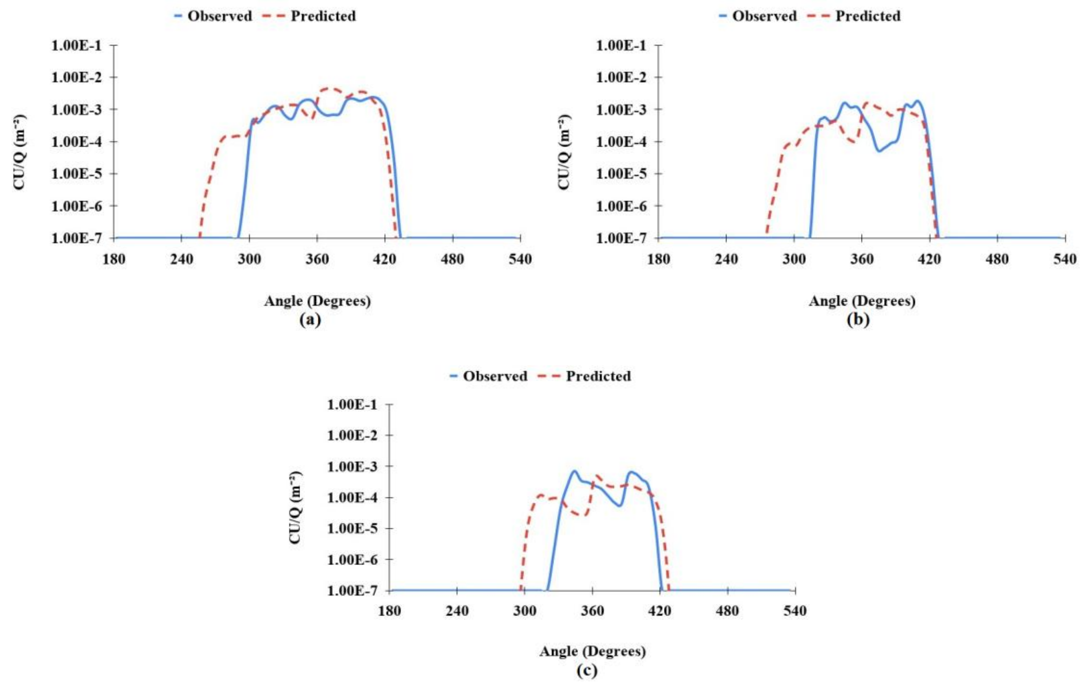

Figure 4. Comparison between observed and predicted SF6 concentration for run 10 at (a) 100m arc, (b) 200m arc and (c) 400m arc

Table 2. Statistical performance measures evaluated for run 10: Normalized Mean Square Error (NMSE), Correlation Coefficient (COR), Factor of Two (FAC2), Index of Agreement (IOA), Fractional Standard Deviation (FS), Fractional Bias (FB), Top 10 Relative Bias (RMB-TT), Geometric Variance (VG) and Geometric Mean Bias (MG)

NMSE	COR	FAC2	IOA	FS	FB	RMB-TT	VG	MG
1.63	0.41	0.375	0.57	-0.52	-0.24	0.59	11.1	0.88

CONCLUSION

This study presents the 3-D CFD simulation for dispersion of a pollutant under low wind stable conditions. The CFD model Code_Saturne® is evaluated with the concentration measurements obtained from a trial of the Idaho Falls field experiment in a flat terrain. The qualitative and quantitative analysis shows that the performance of the model, used in the case of non-homogeneous meteorological conditions, is reasonably acceptable in terms of capturing the multiple concentration peaks and hourly averaged plume spread of the concentration distribution. Also, the anisotropic model predicts ~38% concentrations within a factor of two and overall overestimates the measured concentration. For a better investigation of the model performance, a further study will focus on the simulation of all the test runs of the Idaho Falls experimental campaign. In addition, the sensitivity of the dispersion phenomenon to some physical parameters, such as the height of the release source or turbulence model coefficients, will be considered for future study to improve the numerical predictions.

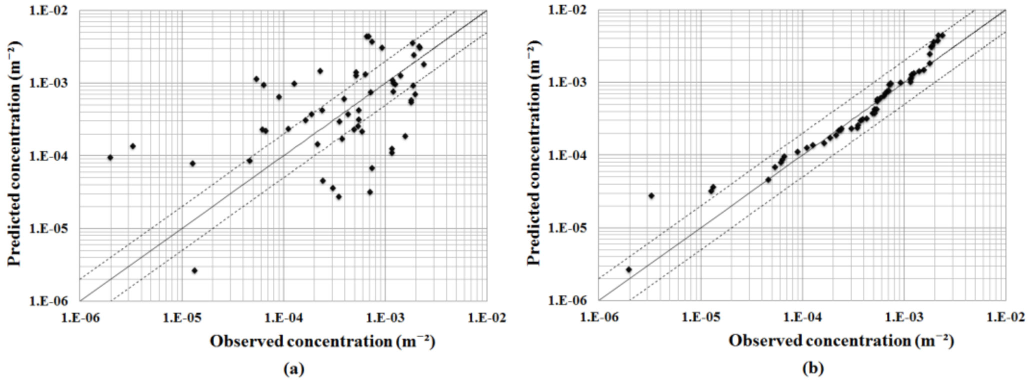

Figure 5. (a) Scatter and (b) quantile-quantile (Q-Q) plot for comparison between observed and modeled concentration for run-10. The dashed lines with offset from the one-to-one solid line represent a factor of two between the observed and predicted concentrations.

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