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AN AIR QUALITY CFD MODEL PERFORMANCE IN COMPLEX ENVIRONMENT WITH EMU OBSERVATIONS

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Abstract: In the frame of this work, the three-dimensional (3-D) computational fluid dynamic (CFD) model fluidyn-Panache dedicated to the dispersion of toxic and hazardous gases around buildings and in geometrically complex chemical sites has been evaluated. The evaluation exercise is based on the following wind tunnel experiments and tracer data from the EMU project (Evaluation of Modelling Uncertainty): A1 (a release from an open door in the courtyard area of a simple L-shaped building on a flat ground) and C1 (a continuous, release over larger distances around an industrial site featuring numerous buildings and complex local topography). A detailed analysis with statistical measures shows that the performance of the fluidyn-PANACHE model against wind tunnel observations with both cases of EMU project is well within the acceptable bounds of statistical measures for air quality applications. The CFD model with three cases A1 and C1 predicts respectively 66% and 67% 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. This study critically examines the real predictive capability of the CFD model fluidyn-PANACHE to apply it in emergency contexts of an accidental or deliberate airborne release in complex environments.

Keywords: *CFD modeling, EMU experiment, fluidyn-PANACHE, Model evaluation, Urban dispersion modelling*

INTRODUCTION

In industrial safety and environment programme, near-field (<10km) dispersion of toxic and hazardous gases near buildings and in a complex chemical site are often predicted with CFD dynamic codes. A CFD model solves the Navier–Stokes equations using a small grid size (of the order 1m or even less) (Hanna et al., 2004) over complex terrain. With rapid advances in computer hardware and methods, CFD models provide now accurate wind flow and dispersion modelling around buildings and other structures in urban areas or industrial areas for any kind of release scenarios. Compared with simple Gaussian dispersion model or other analytical approximations, the CFD model efficiently predict the obstacles influence on wind patterns and cloud shapes (Kumar et al., 2015). Nevertheless, the CFD model evaluation against experimental datasets is one critical point to estimate its capability to provide reliable and valuable informations in emergency planning or chronic impact assessment. Many CFD results were successfully validated against experimental field data (Hanna et al., 2004; Milliez and Carissimo, 2007; Labovský and Jelemenský, 2010). The current paper concerns the fluidyn-PANACHE CFD model evaluation. PANACHE uses physical models and deterministic solutions that are adapted to any kind of release scenarios, complex environments and pollutant characteristics. Here, the evaluation is based on extensive field observations involving tracer gas releases in a wind tunnel from the ‘Evaluation of Modelling Uncertainty’ (EMU) project. EMU provides an unique dataset for evaluation of dispersion models around buildings and over complex topography (Hall, 1997). To demonstrate the PANACHE model’s capabilities to simulate the flow and dispersion patterns in the near field but also at larger distances, the single L-shaped building case and the real industrial site case have been selected.

DESCRIPTION OF THE EMU EXPERIMENT

The ‘Evaluation of Modelling Uncertainty’ (EMU) project funded by the European Commission involves the evaluation of the spread in results due to the way that CFD codes are used and the accuracy of such codes in complex gas dispersion situations. The project consisted in 14 test cases of industrial scenarios were chosen, which ranged from single building on flat terrain scenarios right through to cases associated with a specific, complex topography industrial site. Stage A comprised three cases, Al to A3, involving a simple building on flat ground, neutral atmosphere and isothermal conditions were considered. Stage B incorporated increases in complexity of the geometry (i.e. terrain, obstacles and number of buildings), release conditions (i.e. two-phase and non-isothermal releases) and meteorology (i.e. stability and wind speed). Stage C concerned an actual industrial site, featuring numerous buildings and complex local topography. Experiments were performed at the University of Surrey (Cowan, Castro et Robins, 1995) in a large stratified wind tunnel (20m x 3.5m x 1.5m) at a model scales between 1/133 and 1/250. Continuous jet releases of dense, buoyant and neutrally-buoyant gases have been simulated in neutral or stable atmospheres. In the present work, two test cases A1 and C1 of EMU project have been simulated using commercial software package fluidyn-PANACHE.

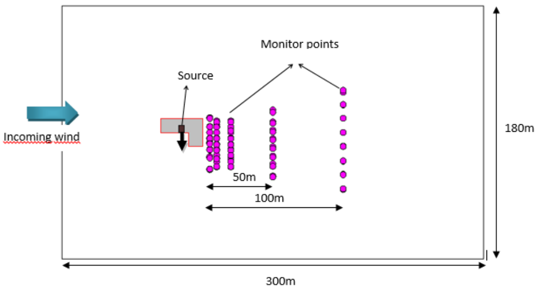

Figure 1. Site features and dimension (Case A1)

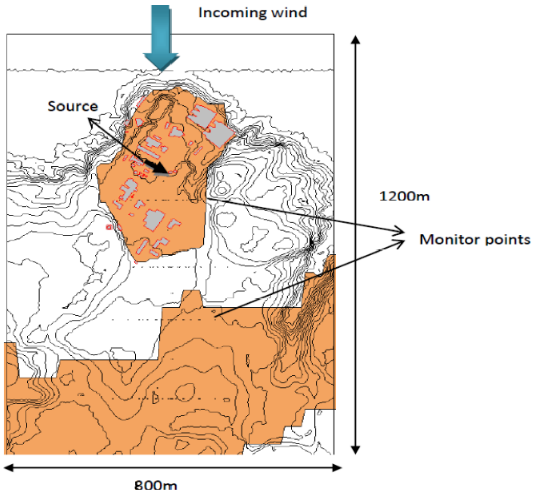

Figure 2. The site features and dimension (Case C1)

SOLUTION AND RESULTS OF EVALUATIONS

EMU project simulation, Case A, Phase I (Case A1)

Case A1 of EMU project entailed the numerical simulation of a passive release from an L-shaped building (see Figure 1) located on a flat surface into an atmospheric boundary layer flow. Neutral ambient conditions were assumed and the EnFlo wind-tunnel was modelled at the University of Surrey. In this case, the concentration predictions at a few cross-wind locations on the cross-section at five distances downwind of the lee edge of the L-shaped building were compared (x_1/H = 0.5, 1, 2, 5, 10; H is the height of the building), corresponding to the numerical simulation sensor positions, are compared with the experimental data. Also, the approximate dimensions of the predicted recirculation zones are compared with observations. Figure 1 represents the computational domain considered for EMU project Case A1. The dimensions have been set as follows: 300 m long, 180 m wide and 120 m high. The distance between the source and the inlet flow boundary condition is 85m and the source is located in the middle of the width of the domain. A mixture of 2.96% ethylene (C_2H_4) in a nitrogen balance was used for the source gas, and was essentially neutrally stable. The properties of the source are listed in Table 1.

Table 1. Source data for the EMU project: Case A1

Type of source	**Exit velocity (m/s)**	**Chemical species**	**Source surface (m²)**	**Height of source (m)**	**Mass flux (kg/s)**	**Temperature (°C)**	**Release duration (s)**
General	1.0	C2H4 (2.96%) N2 (97.04%)	20	2.5	23.68	25	Continuous

The Table 2 contains the comparison of the maximum concentrations for each measurement cross-section in volume fraction with respect to the numerical results. In general, the results are in good agreement with tunnel observations. They are slightly over-predicted where the heights are less than 10m, but slightly under-predicted at the heights more than 10m. The prediction may be assessed, which plot the simulated data against the experimental profiles at $x_1/H=1$, 2, 5 and 10 (not represented here). Close to the building ($x_1/H\leq2$, $z/H\leq1$), the CFD plume is slightly shallower than its experimental counterpart. However, agreement between the simulated and experimental data at sensor positions is very good at a given distance from the source. Figures 3 show the predicted and observed average concentrations comparison for 256 measurement points of case A1 shows good agreement with the wind tunnel observations. One can observe a slight over-prediction tendency in the near field of the release at some locations. The overall simulated concentration predicts 66% of points within FAC2 (Case A1). Also, values of FB, MG, NMSE, NAD and FAC2 are within the acceptable range for each vertical plan.

Table 1. Comparison of modeled and experimental results of ground-level maximum concentration (Case A1) (C/C*)

x1/H	z/H	Exp./Num.
0.50	0.13	4.10E-01
0.50	0.33	4.33E-01
0.50	1.03	6.79E-01
0.50	1.45	1.67E+00
0.50	1.93	1.67E+00
1.00	0.16	4.08E-01
1.00	0.67	6.24E-01
1.00	1.02	8.10E-01
1.00	1.99	1.81E+00
2.00	0.11	4.45E-01
2.00	0.66	5.96E-01
2.00	1.03	9.71E-01
2.00	1.99	1.77E+00
5.00	0.34	6.80E-01
5.00	0.98	9.66E-01
5.00	1.97	1.66E+00
10.00	0.16	9.31E-01
10.00	0.98	1.64E+00
10.00	3.00	1.26E+00

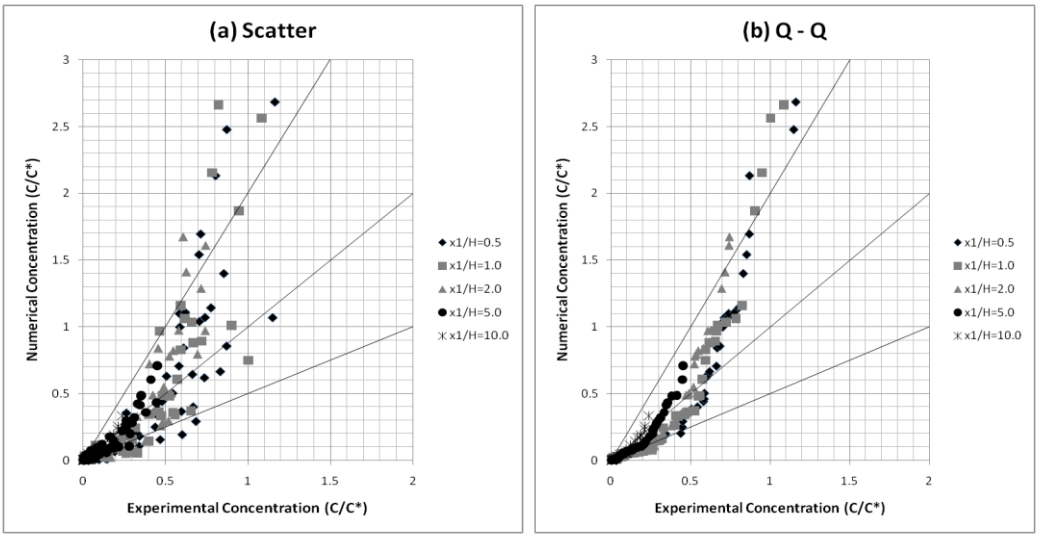

Figure 3. (a) Scatter and (b) quantile-quantile (Q-Q) plots between the predicted and observed average concentrations for 256 points of Case A1. The middle solid line is one-to-one line between observed and simulated concentrations whereas the dotted lines correspond to factor of two.

EMU project simulation, Case C, Phase I (Case C1)

Case C1 of EMU project entails a continuous, passive jet release from the side of a building within a real chemical site. The surrounding terrain is complex, with steep hills, trench-like features and cliffs at the edge of the sea. The site comprises a large number of irregularly shaped buildings, most of which however are conveniently aligned with each other. Cowan (1996) reported the 4 categories of roughness in the domain: sea, land, village/town and industrial site. The atmospheric stability classes encountered are neutral and stable. In this case, we take our origin to be at sea-level, directly below the source position. The source is thus centred on (0, 0, 18.7) m, Three types of concentration data (126 observations) were recorded: cross-stream profiles at ground-level and at (Z-Zg)/H ~ 2-3 (Zg is the height of ground-level), and vertical profiles through the ground-level maxima. A number of other ground-level concentration measurements were also made.

Table 2. Statistical performances measures of the average concentrations for each vertical plan (Case A1)

Criteria	FB	MG	NMSE	NAD	FAC2
Ideal value	0	1	0	0	100%
Acceptable interval	[-0.3 ; 0.3]	[0.7 ; 1.3]	<4	<0.3	>50%
x_1/H =0.5	-0.26	1.22	1.19	0.27	64%
x_1/H =1.0	-0.25	1.21	1.11	0.28	69%
x_1/H =2.0	-0.15	1.29	0.72	0.26	69%
x_1/H =5.0	0.05	1.38	0.21	0.16	63%
x_1/H =10.0	0.13	1.63	0.17	0.14	65%

Hiba! A hivatkozási forrás nem található.2 represents the computational domain of EMU project Case C1.The domain dimensions have been set as 800m long, 1200m wide and 200m high.

Table 4. Source data for the EMU project: Case C1

Type of source	Exit velocity (m/s)	Chemical species	Height of source (m)	Mass flux (kg/s)	Temperature (°C)	Jet direction
Point	7.5	C2H4 (77.3%) N2 (22.7%)	2.0	5.46	15	Horizontal 327.5°

The product released of Case C1 is a mixture of 77.3% by volume C2H4 in N2, giving a mixture density ratio of α = 1.0. The release of C1 is modelled as four point sources. Mass flux, release temperature, release duration, exit velocity and emission direction have been considered as inputs for point model and assumed constant for the release duration. The source characteristics are tabulated on Table 4. Table 5 shows the comparison of modeled and experimental results of ground-level concentration maximum. It is observed that it shows a good comparison with experimental results. The experimental and numerical results for cross-stream profile at ground-level and at (Z-Zg)/H =3.6 are slightly over-predicted at ground-level while they are slightly under-predicted at (Z-Zg)/H =3.6 (not represented here). The vertical concentration profiles in the near-field and in the far-field for Y/H=6.3 and 5.0 have over-prediction tendency at receptors near to the ground-level, however, they are under-predicted at the higher height (not represented here). Accordingly, all performance measures are calculated for each cross-stream profile and each vertical profile separately. The computed statistical indices at each profile are given in Table 6. The variation of FB shows that the extent of under-prediction for each profile and ground-level maxima. Case C1 predicts 66%, 56%, 69%, 75% and100% points within a FAC2 for cross-profile ground-level and (Z-Zg)/H =3.6, vertical profile Y/H=6.3 and 5.0 and ground-level maxima respectively. Also, it predicts 67% of points within FAC2 for the overall simulated concentrations. The simulated averaged concentrations for all 126 observations are presented in form of a scatter plots (Figure 4(a)) and a Q - Q plot (Figure 4(b)). In the scatter plot (Figure 4(a)), it is observed that the simulated averaged concentrations by the

CFD model have good agreement with the observations. The simulated higher averaged 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 averaged concentrations is more visible in Q-Q plot (Figure 4(b)) that shows a comparison of the concentration distributions of simulated and observed concentrations.

CONCLUSIONS

This work presents the 3-D CFD simulations for near-field dispersion of toxic and hazardous gases near buildings and in a geometrically complex chemical site. A CFD model fluidyn-PANACHE is evaluated using two case tests of EMU project: A1 and C1, which ranged from single building on flat terrains right through to case associated with a specific, complex topography industrial site. The simulation was performed in a neutrally stable atmosphere. Quantitative performance measures are used to analyze the performance of the CFD model simulations in 2 cases of EMU project. The overall simulated concentration of case A1 predicts 66% of points within FAC2 for 256 observations. The scatter plots show also good agreement with the wind tunnel observations but the over-prediction tendency at the heights close to ground level. The values of FB, MG, NMSE and VG are within the acceptable range for each vertical plan x_1/H=0.5, 1.0, 2.0, 3.0, 5.0 and 10.0. The simulated results of case C1 shows 100% points within a FAC2 for the ground-level maximum concentrations. Comparison of measured and simulated concentrations for cross-profiles and vertical profiles in the near-field and in the far-field shows the over-prediction tendency at the receptors near to the source but slight under-prediction at far away from the source.

Table 3. Comparison of modelled and experimental results of ground-level maximum concentration (Case C1) (C/C*)

X/H	(Z-Zg)/H	Exp./Num.
5.5	5.0	0.769
11.0	5.6	0.764
11.0	5.1	0.581
19.5	6.0	0.646
30.0	6.3	0.733
30.0	7.0	0.906
37.5	7.0	1.008
45.0	6.8	0.878
45.0	7.0	1.019
56.3	7.0	1.017
67.5	6.8	0.931
67.5	7.0	1.079

Table 6. Statistical performances measures of the average concentrations for each profile (Case C1)

Criteria	FB	MG	NMSE	NAD	FAC2
Ideal value	0	1	0	1	100%
Acceptable interval	[-0.3 ; 0.3]	[0.7 ; 1.3]	<4	<1.6	>50%
(Z-Zg)//H=0 (ground level)	-0.24	3.11	0.59	0.21	66%
(Z-Zg)//H=3.6	0.46	2.12	0.62	1.02	56%
Y/H=6.3	0.05	1.67	0.12	0.12	69%
Y/H=5.0	-0.14	1.32	0.21	0.17	75%
Ground level maxima	-0.27	0.81	-0.20	0.13	100%

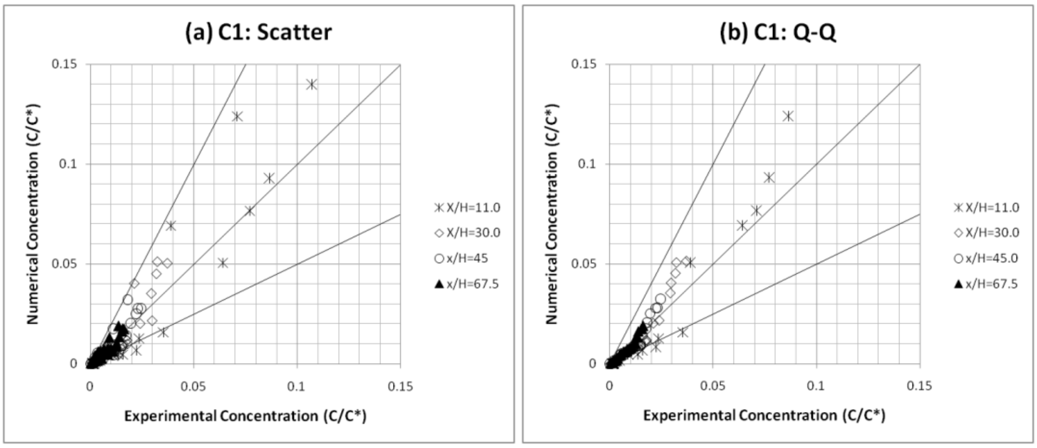

Figure 4: (a) Scatter and (b) quantile-quantile (Q-Q) plots between the predicted and observed average concentrations for 126 points (Case C1). The middle solid line is one-to-one line between observed and simulated concentrations whereas the dotted lines correspond to factor of two.

The values of FB, NMSE, NAD and FAC2 are within the acceptable range for each profile of case C1. Also, it predicts 67% of points within FAC2 for the overall simulated concentrations. The statistical evaluation results show an overall good performance of the CFD model in such complex environment. The CFD model fluidyn-PANACHE used in this study is well suited for the air pollution and emergency planning in industrial or urban areas. This paper is also hoped to share methodologies, contribute to CFD model comparison by collaborative efforts and improve the CFD approaches.

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