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# VALIDATION OF FLUIDYN-PANACHE CFD MODEL AGAINST LARGE-SCALE AND WIND TUNNEL EXPERIMENTS

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**Abstract**: The three-dimensional (3D) computational fluid dynamic (CFD) model Fluidyn-PANACHE dedicated to atmospheric dispersion of toxic and flammable gases has been evaluated in this study. The evaluation exercise is based on the tracer data of the following large-scale field and wind tunnel experiments for dense gases dispersion: Goldfish series (3 trials with 2-phase high-velocity jet releases of acide fluorhydrique (HF) over flat terrain on neutral atmosphere), Coyote series (3 trials with the vertical jet of liquefied natural gas (LNG) on to a water pool with undulations for instable and neutral atmospheric conditions), CHRC series (3 wind tunnel experiments of the dispersion of CO2 over rough surfaces, with and without obstacles on neutral atmosphere), BA-Hamburg tests (3 wind tunnel trials with steady releases of sulphur hexafluoride (SF6) on flat ground, sloping terrain and flat surface with a downwind fence) and BA-TNO tests (3 trials in the wind tunnel facility for vertical releases of sulphur hexafluoride (SF6) over flat and obstructed terrain).
The numerical results are analyzed by the comparison of concentration profiles and scatter plots for five experiments. Moreover, statistical criteria are calculated for quantitative evaluation of the CFD model performance.
Maximum arc-wise concentrations of Goldfish results are slightly under-predicted in the near-field and statistical criteria (shortest averaging) is met for all three cases. Regarding the Coyote series, the results for longest averaging are generally good for most locations of all three cases. For CHRC tests, some under-prediction is observed in the near field for case C. However, the simulated results of maximum arc-wise concentrations agree quite well with the experimental data for cases A and B. For BA-Hamburg tests, the simulated results have slight under-prediction but are well inside the 50% variation interval. The statistical analysis of BA-TNO tests agree well for most locations placed at the source centerline.
Fluidyn-PANACHE predictions have been compared with specific datasets of both the large-scale field trials and the wind tunnel experiments. The statistical evaluation results show the CFD model Fluidyn-PANACHE is capable of simulating the dense gas dispersion in complex situations for industrial and environmental problematics.

***Key words***: *atmospheric pollution dispersion, CFD model evaluation, Fluidyn-PANACHE, dense gas dispersion*

## INTRODUCTION

The air quality and safety have become one of the primary concerns for this century. With the rapid development of computer hardware and numerical methods, the pollution dispersion models, especially 3D CFD model have been used primarily in risk assessment for safety reports in environmental problem and industrial programme since 1990s. The quality of consequence model, especially dense gas dispersion models may be therefore very important to make some decisions for industrial programme.
Compared with simple Gaussian dispersion model or other analytical approximations, the CFD model efficiently predicts the obstacles influence on wind patterns and cloud shapes (Kumar& al., 2015).
Nevertheless, the CFD model evaluation against experimental datasets is one critical point to estimate its capability to provide reliable and valuable information in emergency planning or chronic impact assessment (Hanna & al., 2004; Riddle & al., 2004).
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. To demonstrate the PANACHE model's capabilities with regard of dense gases dispersion in the different accidental conditions, five experimental data set have been selected to evaluate the CFD results: Goldfish series, Coyote series, CHRC tests, BA-Hamburg series and BA-TNO tests.

## DESCRIPTION OF THE CFD MODEL

### Governing Equations

The Fluidyn-PANACHE solves the Navier-Stokes equations along with the equations describing conservation of species concentration, mass, and energy for a mixture of ideal gases. Fluidyn-PANACHE solves the Reynolds averaged forms of these equations for turbulent flow. The Reynolds stresses are modeled using the linear eddy viscosity model (LEVM) (Ferziger and Peric, 2002). Ideal gas law is used for the thermodynamic model of mixture of gases. Air is modeled as moist air with effective properties of the mixture of dry air and water vapor.

### Turbulence Model

Fluidyn-PANACHE uses modified standard k-ε turbulence model to resolve the turbulence structure within the domain. Fluidyn-PANACHE implementation of this model is derived from the standard high-*Re* form with corrections for buoyancy and compressibility (Hanjalic, 2005). It solves the transport equations for turbulent kinetic energy, $k$ and its dissipation rate, $\varepsilon$.

### Boundary Conditions

Boundary conditions are required on the main domain boundary, the ground, and on obstacles. The top boundary is treated as an outflow boundary. The lateral boundaries of the domain are treated as inflow and outflow boundaries based on the direction of the wind with respect to the domain boundary.

### Wind profile

In this study, the log-law profile has been used to parameterize the inflow boundary condition in the three types of atmospheric stability condition: unstable, neutral stable.

### Turbulence profile

The profile selected for this study is a semi-empirical model based on similarity theory and measurements (Han & al., 2000).

## STATISTICAL PERFORMANCE MEASURES (SPM)

Quantitative evaluation of the performance of atmospheric dispersion models requires the definition of appropriate statistical performance measures (SPM) which compare model predictions with measurements. The decision criteria comprise a combination of elements drawn from scientific assessment, the verification process, and the extent to which quantitative values of the SPM output from the validation exercise are also met. Hanna & al. (1993) propose the following modified quantitative assessment criteria to be met by a model:

- A mean bias within $\pm 50\%$ of the mean, corresponding to: -0.4 <MRB<0.4 and 0.67<MG<1.5.
- A scatter of a factor of three of the mean, corresponding to: MRSE<2.3 and VG<3.3.
- The fraction of model observations within a factor of two observations to be at least 50%.

## RESULTS OF EVALUATIONS

### Goldfish series GF1, GF2 and GF3

Three experiments to study atmospheric releases of HF were conducted in 1986 by AMOCO Oil Company and Lawrence Livermore National Laboratory (Hanna & al., 1993). As stated in the report of WP7 of EC URAHFREP, 2001, HF atmospheric dispersion includes different complex behaviors and the molecular weight was modified in order to account for the thermodynamics of HF in air. In the present modelling, HF in polymer form has been selected and the dense gas behavior has been modeled with a 80 g/mol molecular weight.

The results obtained are compared to the experimental data for maximum HF concentration at distances of 300m, 1000m and 3000m in Table 1. The SPM criteria are then applied to the complete set of results available and the statistical evaluation values are shown in Table 2. In all the cases, at all downwind distances the modeled results are under predicting. It may be attributed to the HF, because atmospheric release of HF goes through a rather complicated sequence and changes in molecular weight.

**Table 1.** Comparison of experimental and modeled maximum HF concentrations at different distances downwind

| Distance (m) | GF1 Exp. (ppm) | GF1 Num. (ppm) | GF2 Exp. (ppm) | GF2 Num. (ppm) | GF3 Exp. (ppm) | GF3 Num. (ppm) |
|---|---|---|---|---|---|---|
| 300 | 25473.0 | 17171 | 19396 | 10094 | 18596 | 9069 |
| 1000 | 3098.0 | 3125 | 2392 | 1248 | 2492 | 1217 |
| 3000 | 411.0 | 376 | - | - | 224.0 | 167 |

**Table 2.** BOOT performance criteria for maximum arc wise concentrations for Goldfish series

| Criteria | FB | MG | NMSE | VG | FAC2 |
|---|---|---|---|---|---|
| **Ideal value** | **0** | **1** | **0** | **1** | **100%** |
| **Acceptable interval** | **[-0.3 ; 0.3]** | **[0.7 ; 1.3]** | **<4** | **<1.6** | **>50%** |
| GF1 | 0.33 | 1.17 | 0.35 | 1.06 | 100% |
| GF2 | 0.63 | 1.92 | 0.71 | 1.53 | 100% |
| GF3 | 0.68 | 1.78 | 1.24 | 1.45 | 100% |

## Coyote series CO3, CO5 and CO6

The Coyote trials consist of five experiments for investigation of Rapid Phase Transition (RPT) occurrences (Koopman & *al.*, 1982b). The selected two trials involve the release pool of LNG on plat ground in the unstable and neutral atmospheric conditions.

Figure 1 and Figure 2 show the comparison of modeled and experimental results of shortest (1s) and longest averaging time (90s and 70s respectively for CO5, CO6).
As expected, because of the RANS approach used in PANACHE, the maximum shortest averaging time concentrations are under predicting by factor of two or less in the near-field.
For the longest averaging time concentrations of the Coyote experiments, it has been observed that Fluidyn PANACHE simulations are very good.

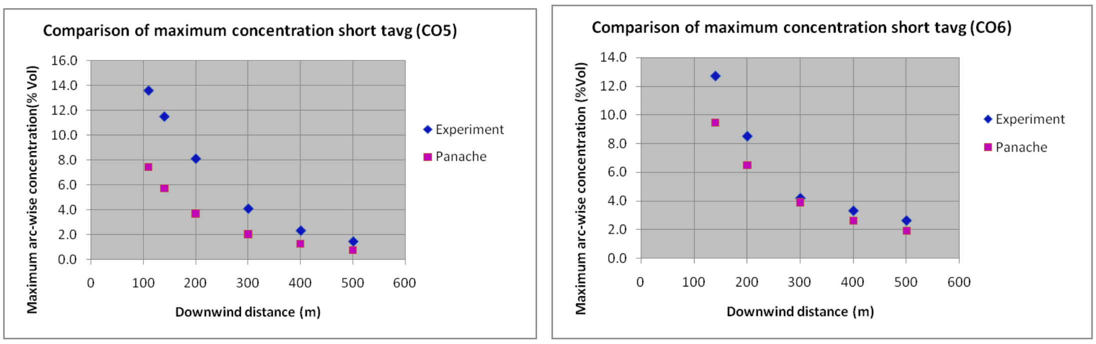



**Figure 1.** Comparison between experimental and numerical maximum arc-wise concentration short time average for CO5 and CO6

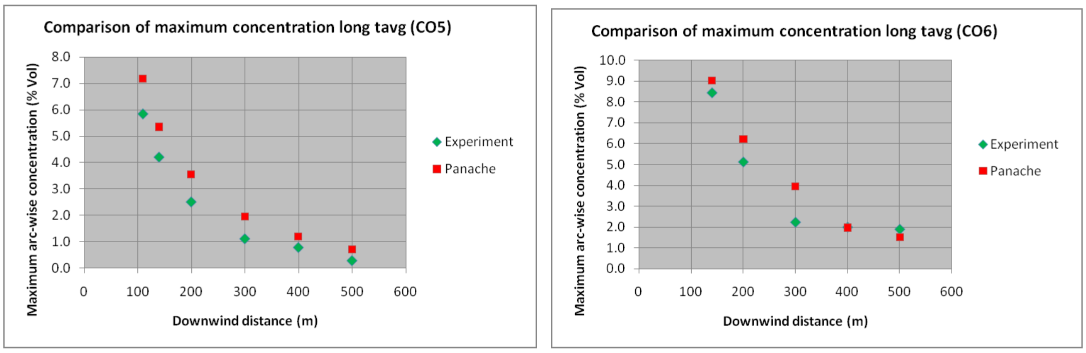



**Figure 1.** Comparison between experimental and numerical (modelled) maximum arc-wise concentration longest time average for CO5 and CO6

### CHRC series Case A, B and C

To provide validation data for the FEM3A dispersion model, the Chemical Hazards Research Center at the University of Arkansas carried out wind tunnel experiments of the dispersion of $CO_2$ over rough surfaces, with and without obstacles (Haven & al., 2007). The PANACHE simulations have been implemented at the equivalent field-scale (150:1 scale) with the presence of roughness elements to comply with CHRC tests reports as shown in Figure 3.

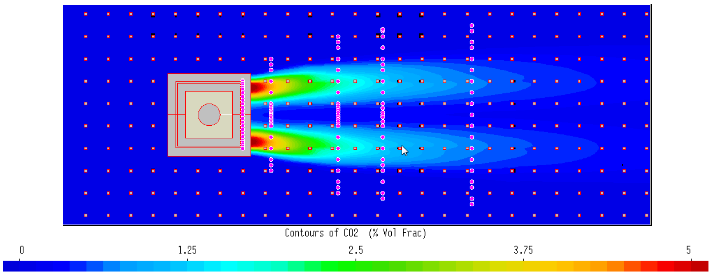


**Figure 2.** Site features and concentration contours (% Vol Frac) on ground level for Case B

Figure 4 shows the experimental and numerical results for lateral concentration profiles at different downwind distances from the source. For cases A and B which includes close field measurements, the predicted cloud at z=0.75m in PANACHE is slightly narrower than in the experiments. For case C, under-predicted values have been observed in the far field.

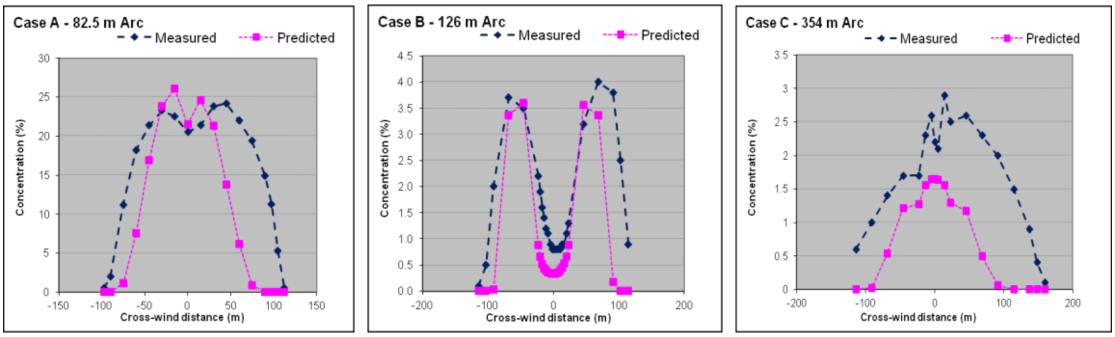
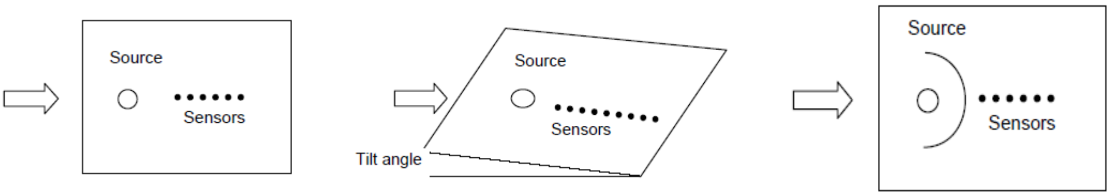


**Figure 3.** Comparison of lateral concentration profiles at different distances downwind

All the SPM results are within the acceptable interval for case A and B. Both cases simulate 100% points within a FAC2. For case C, 57% of the PANACHE predictions are within a FAC2.

### BA-Hamburg Series DA0120, DA0532 and DAT637

The BA-Hamburg trials were conducted in an open circuit wind tunnel at the Meteorological Institute at the University of Hamburg (Nielsen and Ott, 1996). The test cases selected in this study are those that cover the most pertinent configurations.



a) Unobstructed reference case b) Sloping terrain c) Downwind fence

**Figure 4.** BA-Hamburg setup for: a) Unobstructed terrain (DA0120), b) Sloping terrain (DAT637) and c) Downwind fence (DA0532)

The scatter and Quantile-Quantile plots are provided in Figure 6 for steady state results for all the three cases. At most of the points, PANACHE underpredicts the concentration but within the 50% variation interval. The FAC2 of simulated concentrations for cases DA0120, DA0532 and DAT637 are 63%, 70% and 63% respectively.

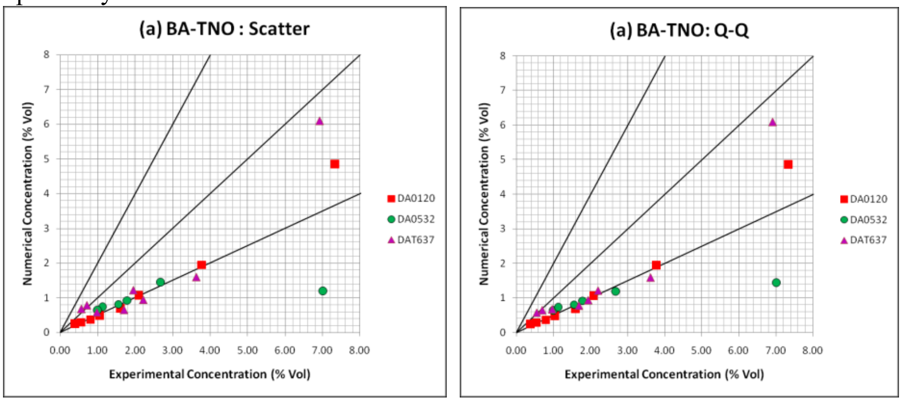



**Figure 5.** Scatter(left) and Quantile-quantile (right) plots for comparison between experimental and numerical results

**BA-TNO Tests**

The experiments were conducted in the TNO "Pollution Industrial Aerodynamics" wind tunnel facility (Rediphem database, 1995). The TUV01 and TUV02 experiments were a 1:78 scale model to investigate the influence of a linear fence perpendicular to the wind direction; The TNO-FLS experiment consisted of a continuous release (over 1000 s) with an unobstructed 3D measurement field.

The scatter and Quantile-Quantile plots are provided in Figure 7 for all three cases.

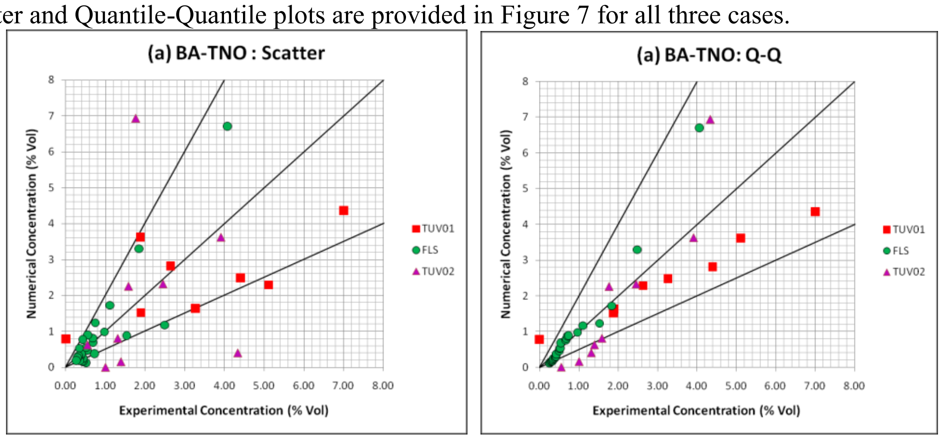



**Figure 6.** Scatter(left) and Quantile-quantile (right) plots for comparison between experimental and numerical results

The vertical concentration profiles at different downstream distances are shown in Figure 8. The simulated concentrations have a under-prediction tendency at receptors near to the ground-level, however, they are well-predicted at the higher height.

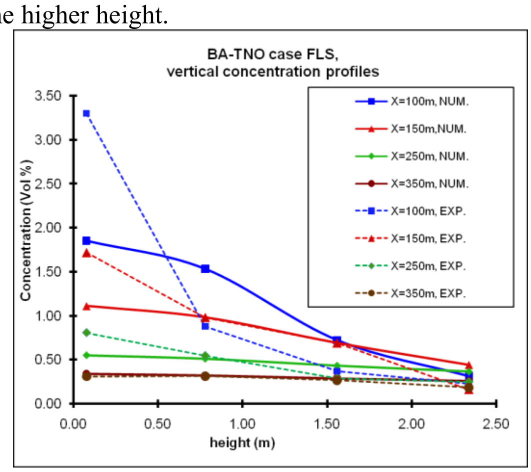



**Figure 7.** Comparison of measured and simulated concentrations for vertical profiles for FLS case

## CONCLUSION

The present study performs a 3D CFD simulation for dense gas dispersion in the atmosphere. A CFD model Fluidyn-PANACHE is evaluated using two series of field-scale tests: Goldfish series and Coyote series, and three series of wind tunnel experiments: CHRC tests, BA-Hamburg tests and BA-TNO tests. The results are analyzed by the comparison of concentration profiles, scatter plots and statistical performance measures.

Maximum arc-wise concentrations of Goldfish data set are underpredicting by a factor of 2 or less. For Coyote series, the results for longest averaging are good for most locations of all two cases (CO5 and CO6), with 83% and 73% points within a factor of 2. For Case A and B of CHRC tests, the simulated results of maximum arc-wise concentrations agree with the experimental data. For BA-Hamburg tests, the simulated results have slight under-prediction but most of the points are within a factor of 2. The FAC2 results of BA-TNO show 75%, 56% and 85% points for TUV01, TUV02 and FLS respectively.

From these experiments, the fluidyn-PANACHE has shown good performance for all the cases considered here and it can be used for dense gas dispersion cases over complex terrain.

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