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VALIDATION OF PANACHE CFD POLLUTION DISPERSION MODELLING WITH DENSE GAS EXPERIMENTS

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Abstract: The prediction of atmospheric pollution dispersion is now one of the first concerns for emergency response and risk assessment. With rapid advances in computer hardware and numerical methods, the computational fluid dynamic (CFD) technology is often applied to determine the consequences of accidental releases of hazardous or toxic materials. The current paper concerns the Fluidyn-PANACHE CFD model evaluation with regard of dense gases dispersion. The CFD model has been evaluated here with four experimental data series for dense gases releases: Desert Tortoise series (4 trials with steady horizontal releases of large scale pressurized liquid ammonia over water surfaces and dry ground), Burro series (4 trials with a liquefied natural gas (LNG) release on a water pool), CO2PIPETRANS series (5 trials with steady and transient leakages of liquid and supercritical CO_2 in a test site), and Porton down series (2 trials with transient releases of a mixture of air and Freon over a flat grassland). The numerical results are analyzed by maximum arc-wise concentration and BOOT criteria for the four experiments. All the simulations of Desert tortoise meet the criteria calculated from the maximum arc-wise concentrations while they have the slight under-prediction tendency far away from the source. Regarding the BURRO series, The BOOT criterion calculated for shortest averaging is met for all the trials in case of flat terrain approach. In the frame of CO2PIPETRANS data series, the comparison of concentration and temperature profiles are in good agreement with the experimental measurements. Concentration time series comparison plots for Porton down series show the good performance of CFD model, with 88% of prediction within a FAC2 of the observations.
This detailed analysis with statistical criteria shows that the performance of Fluidyn-PANACHE model versus these four dense gas experimental data series is well within the acceptable range for air quality applications.

Key words: *atmospheric pollution dispersion, CFD model evaluation, emergency response, dense gas dispersion*

INTRODUCTION

The pollution dispersion models have been used initially in risk assessment for safety reports in environmental problem and industrial programme since 1970s. The quality of consequence model, especially dense gas dispersion models may be therefore very important to make some decisions for industrial programme.

Until now, many dense gas dispersion models have been developped, which range from simple box model through more sophisticated integral models like DEGADIS, SLAB, (Touma et al, 1995) to 3D CFD model (Duijm and Carissimo, 2001). Models for simulating dense gas releases need to account for the source term, initial gravitational spreading of a heavy gas cloud and the downwind dispersion of the cloud in air. With the rapid development of computer hardware and numerical methods, CFD model is becoming increasingly important in this field. Since 1990s, the dense gas CFD models were evaluated by the dense gas release field measurements (Mohan & al., 1995; Duijm et al., 1997; Sklavounos and Rigas, 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 CFD model's capabilities with regard of dense gases dispersion in different accidental conditions even in the most extreme conditions, four field measurements have been selected: Desert Tortoise series, Burro series, CO2PIPETRANS series, and Porton down series. Indeed, evaluation of gas dispersion models need fundamentally to be performed on full-scale releases especially of dense gases to check out the prediction ability.

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. The model 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 compressible, moist with effective properties of the mixture of dry air and water vapor.

Density difference in the vertical direction drives the body force. This model is suitable for flows where density of air changes significantly.

The accuracy of the results produced by a numerical solution procedure in solving the above type of governing equation directly depends on the discretization schemes employed. Accuracy is expressed in terms of the order of a Taylor series expansion used in the discretization of the differential operators in the governing equation.

The TVD (Total Variation Diminishing) scheme is a 2nd order scheme used in the present study.

Turbulence Model

Fluidyn-PANACHE uses a modified standard k-ε turbulence model to solve the turbulence structures with in the domain. The k-ε model is a two-equation linear eddy viscosity model. 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, ε.

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. At the inflow boundary, velocity, temperature and turbulence vertical profiles are specified. Pressure is extrapolated from inside the domain. Species concentrations are set according to the specified background concentrations.

Wind profile

The vertical wind profile is an important choice for the Atmospheric Boundary Layer definition . In this study, a log-law profile based on Monin–Obukhov (M–O) similarity theory has been used to parametrize the inflow boundary condition representative of the atmospheric stability condition: unstable, neutral and stable.

Turbulence profile

Fluidyn-PANACHE has many parametrizations for inlet turbulence profiles. The profile selected for this study is a semi-empirical model based on similarity theory and measurements (Han & al., 2000).

STATISTICAL MODEL PERFORMANCE EVALUATION METHODS

The performance of the CFD model Fluidyn-PANACHE against experimental data is evaluated both qualitatively by results analysis and quantitatively using the standard statistical measures (Chang and Hanna, 2004) such as, Normalized Mean Square Error (NMSE), Fractional Bias (FB), Geometric Mean bias (MG), Geometric Variance (VG) and Factor of Two (FAC2).

For an acceptable model performance, the values of the statistical mesaures must be in the following bounds.

Table 1. BOOT statistical parameters

Parameter	Interval of acceptance	Ideal value
FB	[-0.3 ; 0.3]	0
MG	[0.7 ; 1.3]	1
NMSE	<4	0
VG	<1.6	1
FAC2	Above 50%	100%

RESULTS AND PERFORMANCE EVALUATIONS

Desert Tortoise series 1, 2, 3, and 4

Four large scale pressurized liquid ammonia experiments were conducted during the Desert Tortoise Series in 1983 at the Liquefied Gaseous Spill Test Facility in Nevada (Hanna & al., 1993 and the REDIPHEM database package, 1995).

The experiments were carried out with an 81 to 133 kg sec^{-1} horizontal flash boiling jet source and the duration was from 1 to 8 minutes. The wind speeds were fairly strong from 4.5 to 7.4 $m.s^{-1}$, and the air was dry and hot with 30 –33 °C and 10 –21% relative humidity.

The release configuration for the data assumes a gaseous release, with specific release geometry and flow outlet estimated for a fully expanded virtual jet source at sonic speed. To stay inside the usual practice in industrial assessment cases, the mesh was not further refined.

The maximum experimental concentrations at each range in the downwind direction are considered for the model evaluation.

The table below shows the comparison for each measurement point in volume mass fraction with respect to the numerical results. In most of the cases, the results are in good agreement with experimental results. The results at 100 m are close to experimental while at 800 m they are slightly under predicted at the ground level.

Table 2. Comparison of numerical data with experimental data for Desert Tortoise series (Vol %)

Distance (m)	Z (m)	DT1		DT2		DT3		DT4	
		Exp.	Num.	Exp.	Num.	Exp.	Num.	Exp.	Num.
100	1.0	6.33	6.11	10.958	7.50	9.72	7.75	8.43	7.99
100	2.5	4.78	5.17	7.12	6.54	7.98	6.71	7.09	6.85
100	6.0	-	2.99	3.78	4.31	4.03	4.37	3.89	4.54
800	1.0	1.1	1.09	1.86	1.42	1.56	1.46	2.09	0.96
800	3.5	0.96	0.96	1.71	1.39	1.31	1.31	1.42	0.99
800	8.5	0.29	0.67	0.40	1.20	0.22	0.96		

All the values of FB, MG, NMSE and VG are within the acceptable range as defined in Table 1 and the CFD model predicts respectively 80%, 83%, 83% and 67% points within a FAC2 for the four tests DT1, 2, 3 and 4.

Burro series 3 and 5

The Burro Series of liquefied Natural Gas (LNG) spill experiments were performed at the Naval Weapons Center, China Lake, California during the summer and fall of 1981 (Hanna & al., 1993). Figure 1 represents the computational domain considered Burro tests 3 and 5. First, the undulations near the source are considered.

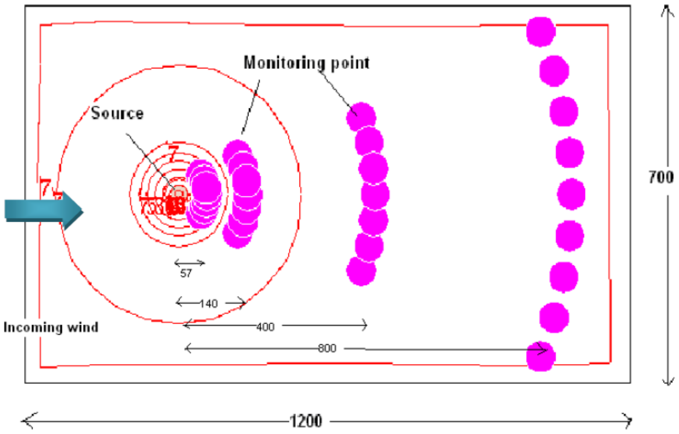

Figure 1. Site features and dimensions for Burro series (m)

Concentration measuring devices are located at 57, 140, 400 and 800 m distance from the source. The meteorological data included wind, turbulence and temperature measurements to describe the turbulent atmospheric boundary layer. For modelling purposes, total mass flow rate from the pool is assumed to be equal to release rate as pool spreading and vaporization reach equilibrium with the release rate.

The following figures show the area occupied by instantaneous cloud contours with the scale of 1%, 2%, 5%, 10% and 15% over the domain at 1m height. These areas are calculated at 50s and 190s and are compared to the experiment data (area of cloud contour). The modelled results are slightly under-predicting for 1% and 2% and over predicting for 5%, 10% and 15%.

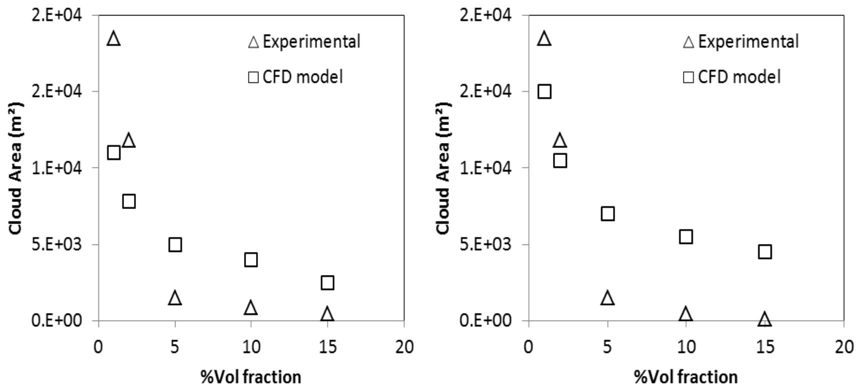

Figure 2. Comparison of surface area with experimental results at 50 secs (left) and at 190 secs (right) of BU5 case

The comparison of modeled and experimental results of shortest (1s) and longest averaging time for BU3 (100s) and BU5 (130s) is shown in Table 3. The shortest averaging time results are under-predicted because of the RANS model used in the CFD model while the longest averaging time results are over-predicted at 57 m and slightly under-predicted at 140 m. The longest averaging time results at 140 m for BU5 experiment shows very good agreement. The unsteady solution predicts more than 50% points within factor of two for the both experiments.

Table 3. Comparison for maximum arc-wise LNG concentration (ppm) for shortest and longest averaging from different downwind distances at 1m height

Distance (m)	BU3				BU5			
	Longest (100s)		Shortest		Longest (130s)		Shortest	
	Exp.	Mod.	Exp.	Mod.	Exp.	Mod.	Exp.	Mod.
57	79053	125363	224380	126245	68925	137401	190410	137854
140	63731	33581	8 9850	33749	49913	47174	96000	47377

CO2PIPETRANS series T5DS1, T8 DS1, T11DS1 and T14DS2

To investigate and fill the identified knowledge gaps and to validate computer dispersion models for liquid and supercritical CO_2 releases, BP set up a research project in 2006. This section covers the validation of dispersion results obtained by PANACHE against the experimental results for both high-pressure cold release and high-pressure supercritical release.

Table 3. Discharge data for T5DS1 and T11DS1 cases

Discharge data	T5	T11
Inlet pressure (bar)	156.9	82.2
Inlet temperature (°C)	12.5	18.4
Orifice diameter (mm)	25.4	12.7
Steady/transient	steady	steady
Mean mass flow rate (kg/s)	40.7	7.1

In the frame of this validation case, source term was modeled as Pseudo source (temperature, pressure, velocity…).

For many sensors, concentrations levels are not constant but vary significantly with time over the period of CO_2 injection. Steady state simulations with RANS approach gives unique value at converged state.

Steady cases T5DS1and T11DS1

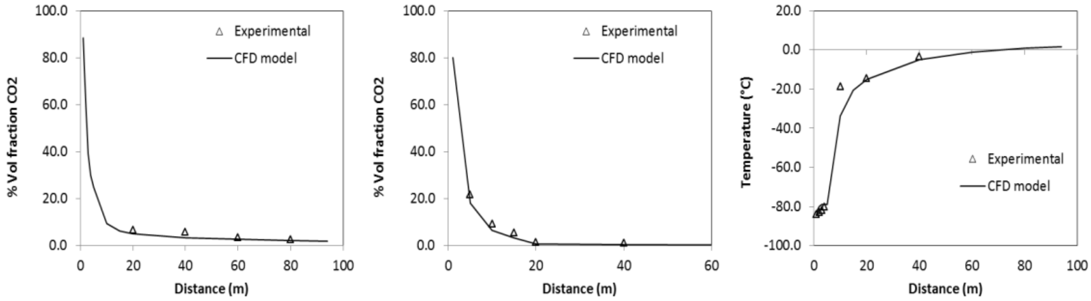

Figure 3. Concentration of CO_2 at 1m height from the ground along the axis of leak at different downwind distances from the source for T5DS1 (left) and T11DS1 (center) (sensors accuracy ±1%) - Temperature at 1m height from the ground along the axis of leak at different downwind distance from the source for T5DS1 (right)

The CO_2 concentration is well predicted in the near and far field form the release section.

Transient cases T8DS1 and T14DS2

Time varying mass flow rate at the source point has been modelled. The results obtained for hot T08DS1 and cold T14DS2 releases are shown in Figure 4 for concentration comparison with the experimental results.

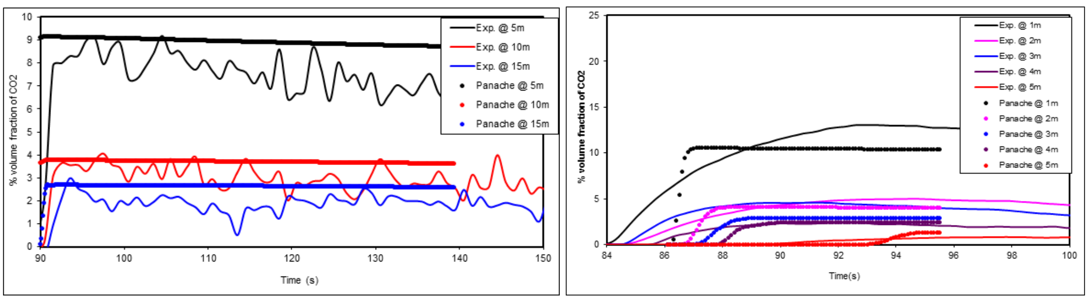

Figure 4. Temporal concentration of CO_2 at 1m height along the axis of leak at different downwind distances from the source for T8DS1 (left) and T14DS2 (right) (sensors accuracy ±1%)

Porton down series 26 and 29

Forty two moderate scale (40 m^3) Freon (CCl_2F_2) dispersion experiments "Porton Down Series" were conducted in 1976 at the Chemical Defence Establishment in Porton Down (Picknett Report, 1978). The simulation results for trial No. 26 are compared with field trials and the results of No. 29 are compared with wind tunnel results trials (Hall et al, 1982).

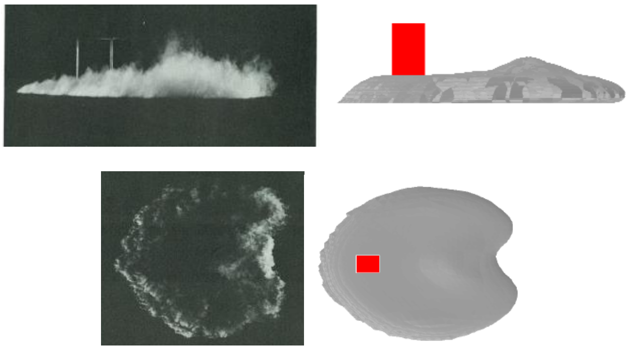

Figure 5. CFD modeled and wind tunnel modeled top view visualisation comparison for trial 29 at 4.3 sec

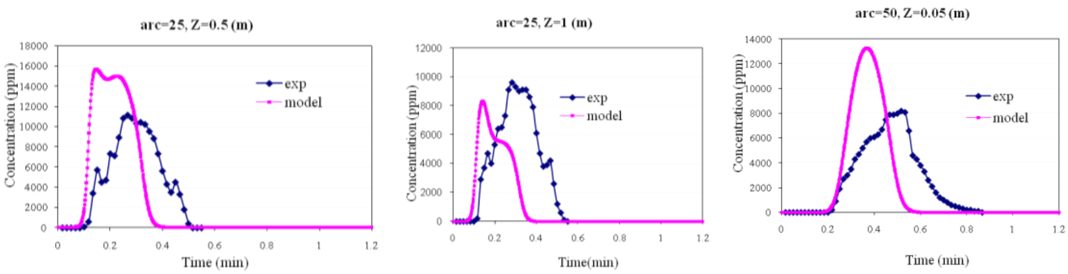

Figure 6. Concentration time series comparison plot for trial no 26

In general, the simulations results show good agreement with field trials at the different sensor locations. The cloud arrival times are also in very good agreement but cloud departure times are slightly under-predicted.

CONCLUSION

The present paper shows the CFD model Fluidyn-PANACHE evaluation in four dense gases releases experiments: Desert Tortoise series, Burro series, CO2PIPETRANS series, and Porton down series. The results are analyzed for maximum arc-wise concentration and standard statistical criterion.

For these experiments, the CFD model has shown good performance for all the cases. It can be used with confidence in contexts of various dense gas accidental releases.

REFERENCES

Duijm, N.J. and B. Carissimo, 2001: Evaluation methodologies for dense gas dispersion models. In: (ed.: M. Fingas) The handbook hazardous materials spills technology. Mc Graw-Hill, New York.

Duijm, N.J., B. Carissimo, A. Mercer, C. Bartholome and H. Giesbrecht, 1997: Development and test of an evaluation protocol for heavy gas dispersion models. *J. Hazard. Mater*., **56**, 273-285.

Ferziger, J.H. and M. Perić, 2002: Computational Methods for Fluid Dynamics. Springer.

Hall, D.J., E.J. Hollis and H. Ishaq, 1984: A wind tunnel model of the porton dense gas spill. In: (eds: Ooms, G. and Tennekes H.) Atmospheric Dispersion of Heavy Gases and Small Particles. Symposium, Delft, The Netherlands August 29 – September 2, 1983. Springer.

Han, J., S.P. Arya, S. Shen, and Y-L Lin, 2000: An Estimation of Turbulent Kinetic Energy and Energy Dissipation Rate Based on Atmospheric Boundary Layer Similarity Theory. NASA/CR-2000-210298.

Hanjalic, K., 2005: Turbulence And Transport Phenomena: Modelling and Simulation. Turbulence Modeling and Simulation (TMS) Workshop, Technische Universität Darmstadt.

Hanna, S.R., D.G. Strimaitis and J.C. Chang, 1993: Hazard Response Modeling Uncertainty (A Quantitative Method). Volume 2. Evaluation of Commonly Used Hazardous Gas Dispersion Models. SIGMA RESEARCH CORP WESTFORD MA.

Kohout, A. J., 2011: Evaluation of fire dynamics simulator for liquefied natural gas vapor dispersion hazards (Doctoral dissertation).

Mohan, M., T.S. Panwar and M.P. Singh, 1995: Development of dense gas dispersion model for emergency preparedness. *Atmos. Environ*., **29**, 2075-2087.

Picknett, R.G., 1978: Field Experiments On The Behaviour Of dense clouds, main report. Report 1 and 2 (d), 3(b),(c), Chemical Defence Establishment.

Rediphem database, 1995: A Collection of Data from Dense Gas Experiments. Morten Nielsen and Søren Ott, Risø Laboratory Report: Risø-R-845(EN), ISBN 87-550-2113-1.

Sklavounos, S. and F. Rigas, 2004: Validation of turbulence models in heavy gas dispersion over obstacles. *J. Hazard. Mater*, **208**, 9-20.

Touma, J.S., W.M. Cox, H. Thistle, J.G. Zapert, 1995: Performance Evaluation of Gas Dispersion Models, *J. Appl. Meteorol*., **34**, 603-615.