VALIDATION OF FLUIDYN-PANACHE CFD DISPERSION MODEL WITH DENSE GAS EXPERIMENTS



FLUIDYN

Software and studies – R&D

- Computational fluid dynamics (CFD)
- Multiphysics coupling (Fluids, Structures, Heat transfer etc.)

Domains of activities :

- Historically : Aeronautics, energy
- Nowadays : Environmental impact, Industrial hazards

Main software :

- fluidyn-MP : general multiphysics platform
- Fluidyn-PANACHE : platform dedicated to atmospheric dispersion



FLUIDYN-PANACHE

- Developed since 1993
- Pollutant dispersion in atmosphere for environmental impact and industrial hazards
- CFD Eulerian solver (Finite Volumes) RANS formulation (k-epsilon model)
- Dedicated preprocessing, meshing, solver, and post-processing









WORKING GROUP ON CFD IN DISPERSION

- Increased use of CFD in regulatory studies but lack of experience of inspectors
- Working group requested by the French Ministry of Environment
- Headed by INERIS
- Joined by : industries, consultancy groups, software editors and researchers
- 3 subgroups :
 - Theory
 - Tests and trials
 - Dissemination
- Guidelines published in September 2015



DENSE GAS VALIDATION CASES

Case	Product	Windspeed	Source	Mass flow rate
Desert Tortoise	Ammonia	4.5 - 7.4 m/sec	Jet	81-133 kg.sec ⁻¹
Burro	LNG	5.4 - 7.4 m/sec	Pool	11 to 18m ³ /min
CO2PIPETRANS	CO ₂	5.5 – 6.0 m/sec	Jet	4 – 40 kg.sec ⁻¹
Porton Down	Freon	4 – 4.7 m/sec	Instantaneous release	40 m ³



PERFORMANCE EVALUATION

- Qualitatively by results analysis and shape of cloud
- Quantitatively :
 - By direct comparison of maximum concentration values
 - By the standard statistical measures (BOOT Chang and Hanna, 2004)
 - Normalized Mean Square Error (NMSE), Fractional Bias (FB), Geometric Mean bias (MG) Geometric Variance (VG), Factor of Two (FAC2).

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%

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DESERT TORTOISE SERIES - SIMULATION

- 4 tests out of the REDIPHEM database conducted by LLNL
- Desert set-up





Sample of ground-level velocity vectors at the release point



DESERT TORTOISE SERIES - ASSESSMENT

- The results at 100m are close to experimental while at 800m they are slightly under predicted at the ground level.
- All the values of FB, MG, NMSE and VG are within the acceptable range
- FAC2 between 67 and 83%

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BURRO SERIES - SIMULATION

- 2 tests from REDIPHEM database conducted by NWC and LLNL
- Desert set-up with a steep slope at the source (pool)

BURRO SERIES - EVALUATION

- Instantaneous area cloud contours compared to the experimental
- Slight underprediction for MF 1% and 2% and overprediction for 5%, 10% and 15%.
- Most of BOOT criteria are within acceptable ranges

	BU3			BU5					
Distance (m)	Longest (100s)		Shortest		Longest (130s)		Shortest		
	Exp.	Mod.	Exp.	Mod.	Exp.	Mod.	Exp.	Mod.	
57	79053	125363	224380	126245	68925	137401	190410	137854	m
140	63731	33581	89850	33749	49913	47174	96000	47377	

CO2PIPETRANS SERIES - SIMULATION

• 5 cases from BP and Shell datasets available from DNV website

CO2PIPETRANS SERIES - EVALUATION

• CO₂ concentration and temperature is well predicted in the near and far field form the release section.

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PORTON DOWN SERIES - SIMULATION

- 3 tests conducted by Chemical Defence establishment and HSE
- 2 tests done in wind tunnel experiments as well
- Flat terrain

PORTON DOWN SERIES - EVALUATION

CONCLUSION

- CFD model Fluidyn-PANACHE evaluation in four dense gases releases experiments: Desert Tortoise series, Burro series, CO2PIPETRANS series, and Porton down series.
- Test cases not designed for CFD
- 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.

GUIDELINES

- 1. Validation of the numerical tool
- 2. Atmospheric stability class conservation over a 2-km domain
- 3. Grid independency
- 4. Proper meshing of obstacles (10 cells)
- 5. Cell aspect ratio less than 10
- 6. Mesh orientation aligned with the wind
- 7. Numerical scheme of at least 2nd order of precision
- 8. Growth factor less than 1.2 between two cells
- 9. Wind profiles as defined by the WG
- 10. Boundary conditions far from zone of interest
- 11. Proper integration of the source term (geometry, temperature)
- 12. Modification of the wind field by the source, if applicable
- 13. Prandtl and Schmidt numbers equal to 0.7
- 14. Proper turbulence model

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