Evaluation of DISPAL CFD model against Prairie Grass and Kit Fox Field dataset for neutral to stable atmospheric conditions

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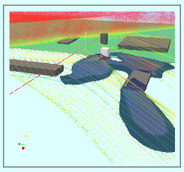
Context



DISPAL is an eulerian CFD model using RANS / URANS approach to model atmospheric dispersion. It is:

✓ Used for consequences assessment of gaseous dispersion within Air Liquide Group

✓ Recognized by French regulatory authorities as Air Liquide 3D model to take into account obstacles on dispersion

→ Continuously enhanced and evaluated following standard procedures since 25 years

→ Recent focus on neutral to stable conditions

General settings:

✓ Standard k-ε turbulence closure model with specific treatment of $C_{3\varepsilon}$ and Pr_t constants to take into account buoyancy effects (partly based on [Alinot and Masson, 2005])

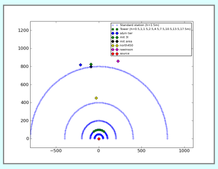
✓ Wind and temperature profiles based on Monin-Obukhov similarity theory used to specify inlet and initial conditions

✓ Turbulent quantities profiles based on production-dissipation balance assumption

✓ Statistical parameters for performances evaluation exercise issued from [Chang & Hanna, 2004]:

→ MG: geometric mean bias, VG: geometric variance, FB: fractional bias, NMSE: normalized mean square error, FAC2: fraction of predictions within a factor two of observations

Project Prairie Grass



Objectives

✓ **Validate the enhanced capability of DISPAL to maintain turbulent profiles along the computational domain for neutral to stable conditions**

✓ **Investigate the influence of Schmidt turbulent number on dispersion modeling**

Information

✓ Diffuse passive tracer dispersion over a flat terrain

✓ Pasquill-Gilford classification built on energy budget method and wind profile reconstruction

✓ Trials excluded from the panel: 14, 32, 53, 58, 59

✓ Statistics performed for criteria

- C_{max} (arc-wise maximum concentration),
- C_y (cross-wind integrated concentration)
- σ_y (cross-wind standard deviation)

Conclusions

✓ Deterioration of statistics with increasing distance (in part due to low-frequency fluctuations effect)

✓ General trend to overestimation

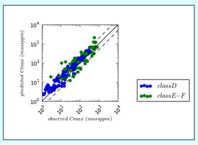
✓ Best performances observed for neutral conditions but results for stable conditions improved compared to the previous DISPAL version

✓ Performances highly affected by Schmidt number value

→ Schmidt number around 0.7 gives better performances for all classes (results showed here)

Nevertheless, a good level of performances is reached

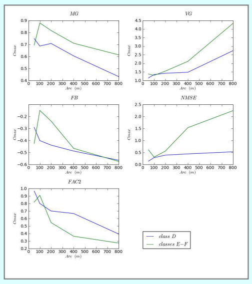
Main results

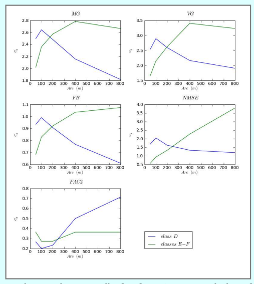


Scatterplot for C_{max} criteria

	MG	VG	FB	NMSE	FAC2
C_{max}	0.74	1.48	-0.35	0.98	0.67
C_y	1.48	1.31	0.34	0.44	0.67
σ_y	2.37	2.45	0.87	1.57	0.30
Criteria	0.7 < MG < 1.3	< 1.6	-0.3 < FB < 0.3	< 4	> 0.5

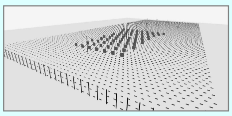
Overall statistics





Statistical performances according to the distance from the release (left: for C_{max} ; right: for σ_y)

Kit Fox Field



Objectives

✓ **Validate the capability of DISPAL to handle heavy gas dispersion for various atmospheric stability conditions and for continuous and puff releases**

Information

✓ CO_2 ground diffuse release on a rough area

✓ All trials simulated (URA & ERP / Continuous & Puff releases)

✓ Schmidt number sensitivity investigated

✓ Mesh sensitivity investigated (results showed on a 1M points mesh)

✓ Implicit roughness used for ERP trials

✓ Statistics based on dose quantity

Conclusions

✓**Good level of performances reached for continuous releases**

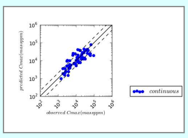
✓Significant underestimation of lateral cloud speeding for puff releases

✓Better agreement for URA trials → ERP roughness need to be explicitly modeled or a larger roughness length is more suitable

✓Schmidt number = 0.7 gives better performances

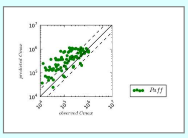
Main results for Cmax criteria

Continuous trials



	MG	VG	FB	NMSE	FAC2
25 m	1.13	1.71	0.18	0.47	0.62
50 m	1.03	1.52	0.08	0.32	0.67
100 m	1.02	1.41	0.08	0.32	0.72
225 m	0.79	4.95	-0.03	0.13	0.89
global	1.02	1.60	0.08	0.32	0.73

Puff trials



	MG	VG	FB	NMSE	FAC2
25 m	0.62	2.1	-0.4	0.51	0.61
50 m	0.42	4.01	-0.73	1.21	0.53
100 m	0.3	6.20	-0.98	1.62	0.31
225 m	0.3	16.14	-0.99	2.55	0.22
global	0.36	5.15	-0.85	1.41	0.42

Conclusions

→ An extended validation of DISPAL for the modeling of passive and heavy gas dispersion in stably stratified atmospheric boundary layer has been positively achieved

→A further model validation for elevated heavy gas releases is expected

References

- Alinot C. and Masson C., 2005, *k-ε model for the atmospheric boundary layer under various thermal stratifications,* Journal of Solar Energy Engineering, vol 127, 438 – 443
- Chang J.C. and Hanna S. R., 2004, *Air quality model performance evaluation,* Meteorology and Atmospheric Physics, vol. 87, 167 - 196