MICROSPRAY SIMULATION OF DENSE GAS DISPERSION IN COMPLEX TERRAIN

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An updated version of the Lagrangian particle dispersion model

MicroSpray

recently adapted to study dense gas dispersion and its interaction with obstacles, if any, is presented.

Three tests were carried out:

1) simulation of a real field accident (the Macdona railroad accident in USA, with emission of huge amounts of chlorine);

2) simulation of the Kit Fox tracer experiments

3) comparison between MicroSpray and CFD Mercure simulations of dispersion in presence of obstacles

Model system **MSS**

MicroSwift

prognostic (mass consistent) wind interpolator over complex terrain accounting for complex terrain and buildings

MicroSpray

LPD model derived from SPRAY; it accounts for the presence of buildings, other obstacles, complex terrain, and possible occurrence of low wind speed

Mercure

(Carissimo et al., 1997) is the atmospheric adaptation of the CFD code ESTET developed by Electricité. de France (EDF), commonly used for industrial CFD applications at EDF R&D.

Relevant aspects of the code include: 3-D flow simulation, influence of terrain and obstacles, multiple fluids and full non-hydrostatic formulation.

Mercure solves the classic Navier-Stokes equations system with adaptations for multiple fluids and for passive scalar tracer variables.

Solving the thermal energy equation implies that thermal buoyancy (or dense) effects are included in the solution.

Chlorine accident - Macdona, TX, USA

June 28, 2004 two trains collision

Picture from *Railroad Accident Report NTSB/RAR-06/03*

We refer to a Report by **Hanna, S.R**. (2007)

in which the simulations by six widely-used hazardous gas models

SLAB, HGSYSTEM, ALOHA, SCIPUFF, SAFER/TRACE, PHAST

of three recent railcar accidents in USA were compared

Being accidents that occurred at remote locations, no meteorological and concentration observations are available,

thus source emission rates were estimated and it was not possible to state which model was "best"

It was concluded that the **six models agree** in their estimate of the downwind dispersion within **one order of magnitude**

Chlorine accident - Macdona, TX, USA

Emission was estimated to last 136 s, dispersion simulations lasted 30 minutes

A computation domain of 2,200 m x 1,400 m x 1,000 m was considered.

100 particles were released per second from the 1 m source.

Concentration was computed at 60 fictitious samplers per arc

at the downwind distances (0.1, 0.2, 0.5, 1 and 2 km)

We computed the following quantities:

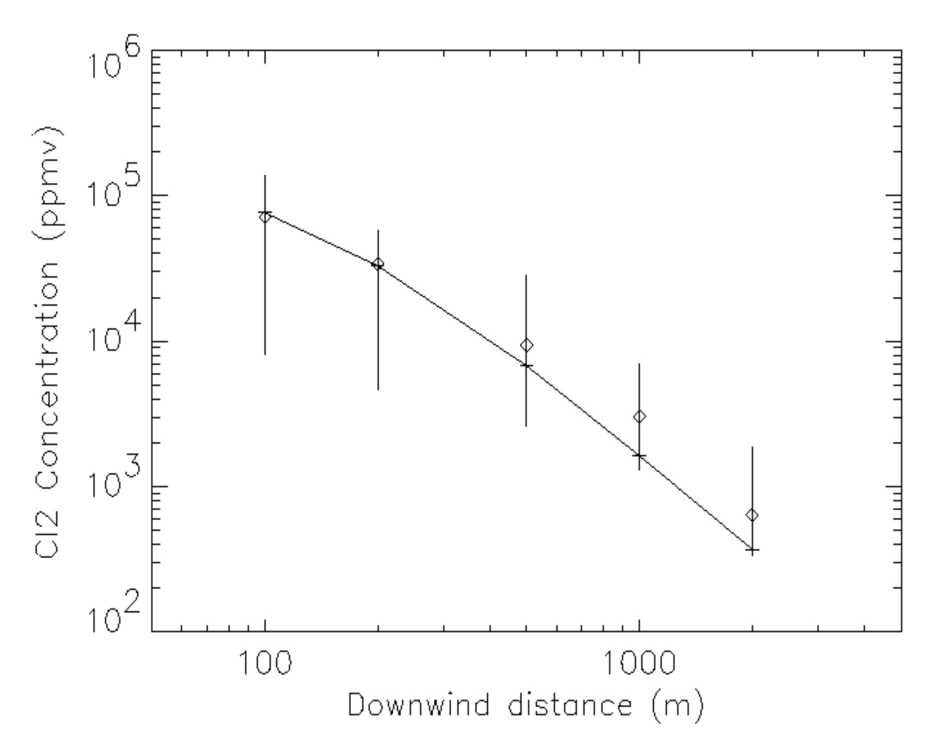
max model-simulated 10 min average Cl_2 concentration at the above 5 arcs,

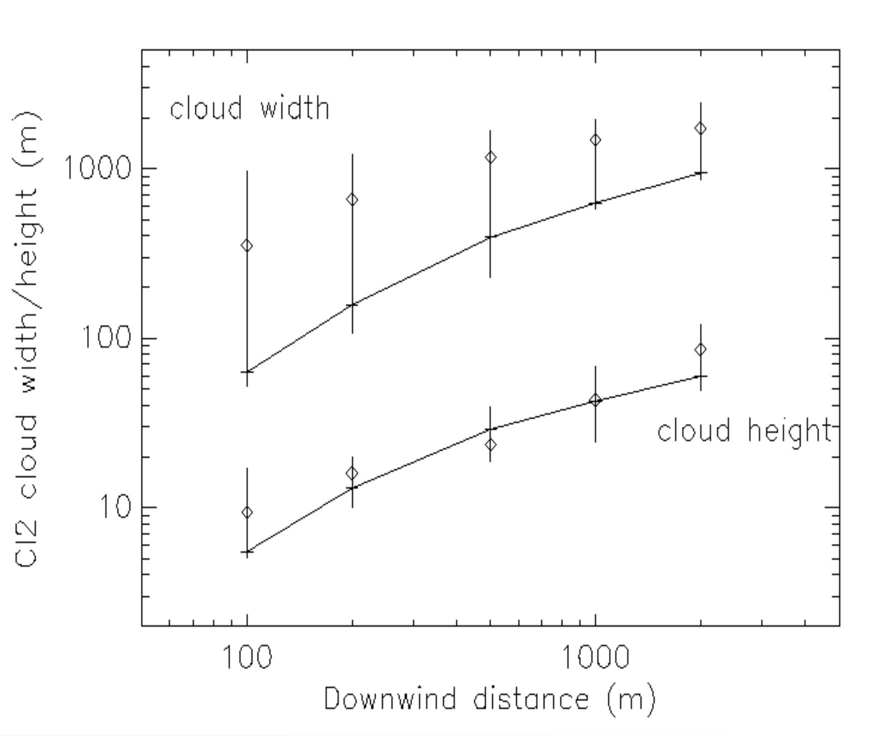
plume width

plume height

} **to the model-simulated conc. of 2000, 400, and 20 ppm at the 5 arcs**

MSS results compared to the **Macdona accident** simulations from six widely-used models (Hanna, 2007). Continuous lines indicate present results, vertical bars show the variability (max, min) of the six models, circles locate their median





Left graph refers to the **Cl2 concentration versus distance**; right graph plots **Cl2 cloud width and height**, both to the model-simulated concentration of 20 ppm versus distance

Lacking direct observations it is not possible to rank the seven (six plus MSS) model results.

Results shown indicate that MSS is as accurate as the ensemble of six widely used models.

It was also verified that the concentration, C, varies with distance, x, according to

$$C_2/C_1 = \left(x_2/x_1\right)^{-p}$$

with p = 1.54, that is in the expected range: 1.5 – 2 (Britter et al, 2002)

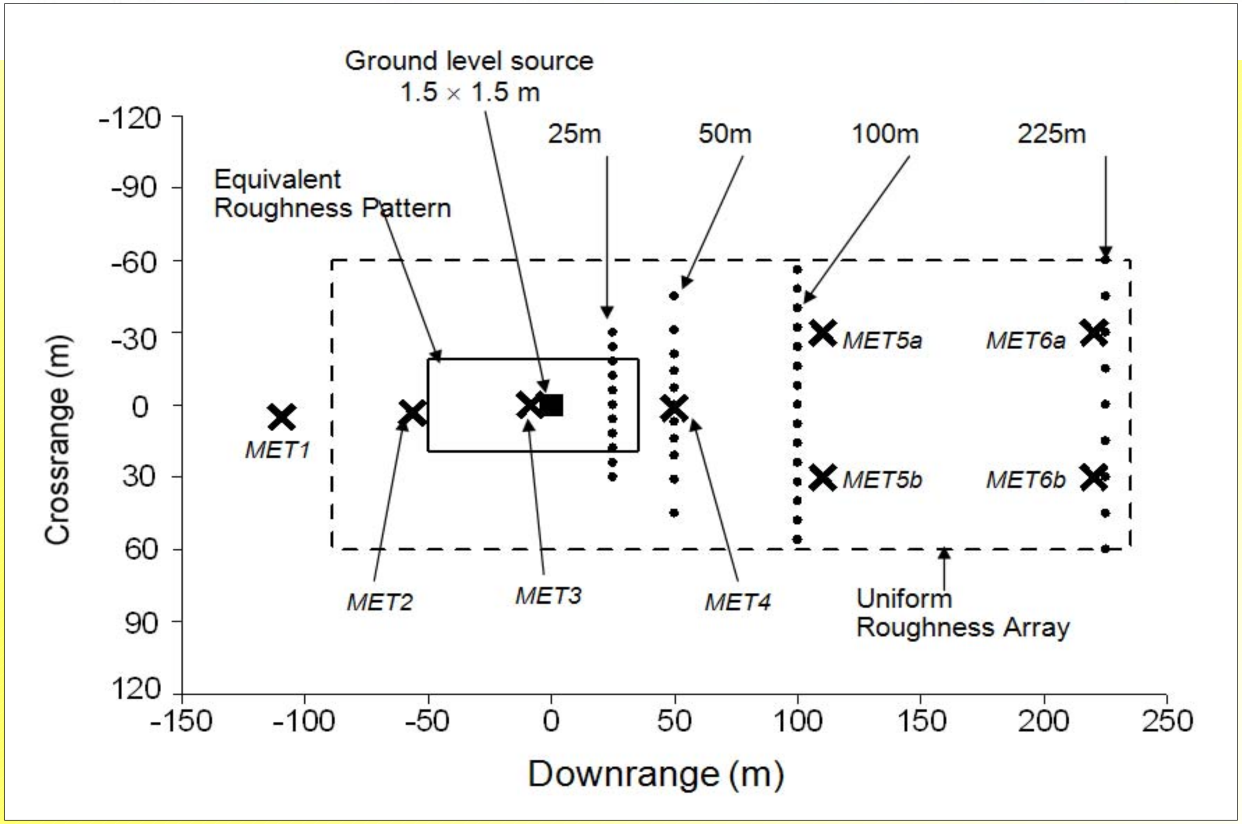
Kit Fox dense gas field data set overview

- The Kit Fox experiment was performed in 1995 at the US Department of Energy (DOE) Nevada Test Site.
- It consists of 52 trials where CO_2 gas releases were made at ground level during neutral to stable conditions (both « puffs » and « continuous plumes » releases were performed).
- Experiments were carried out for a uniform surface roughness of 0.01/0.02 m (URA) and also using an increased surface roughness of 0.12/0.24 m in the neighbourhood of the source (ERP).
- Fast response concentration monitors (one reading per second) were installed at four downwind arcs (25, 50, 100, and 225 m). Meteorological instruments where installed on 5 towers.

Kit Fox dense gas field data set overview

- The Kit Fox experiments are split into four groups:
- ERP - Puff: 13 experiments, of which 2, 7, 3 for stability D, E and F respectively
- ERP - Continuous: 6 experiments, of which 1, 1, 4 for stability D, E, and F respectively
- URA - Puff: 21 experiments, of which 8, 5, 8 for stability D, E, and F respectively
- URA - Continuous: 12 experiments, of which 2, 7, 3 for stability D, E, and F respectively

Plot plan of the Kit Fox site



Validation of MSS against Kit Fox field data

- The 52 trials have been modeled using Mspray
- Uniform roughness lengths have been considered, at the moment, for URA and EPR simulations (0.015 and 0.18 m respectively).
- Only a single meteorological data, at 2 meters above ground level, has been considered per trial (MSwift has not been used in order to interpolate data from different profiles).
- Instantaneous concentrations every second have been saved when running MSpray. Comparisons between observations and simulations have been performed using a 20 seconds averaging time, at each downwind arc (maximum concentrations).

Validation of MSS against Kit Fox field data

- Friction velocity, Monin Obhukov's length, roughness length as well as Pasquill-Gifford stability class were provided as inputs.
- Mixing layer heights have been estimated using methodology from the Yellow Book of TNO.
- Lagrangian turbulence has been internally generated by MSpray thanks to these previous parameters: sonic anemometers data have not been considered yet.
- Vertical profiles of wind speed have been generated thanks to Irwin power laws (based on Pasquill-Gifford stability class and wind speed at 2 m above the ground level).

Validation of MSS against Kit Fox field data

Statistical evaluation of comparisons between observations and predicted data includes:

geometric mean bias (MG),

geometric variance (VG)

factor of 2 (FA2)

Kit Fox experiment	Overall	URA Continuous	URA Puff	ERP Continuous	ERP Puff
	52 experiments	**12 experiments**	**21 experiments**	**6 experiments**	**13 experiments**
MG	1.04	1.42	0.95	1.19	0.87
VG	1.20	1.20	1.15	1.25	1.29
FA2	88 %	92 %	99 %	83%	83 %

Validation of MSS against Kit Fox field data

- Results obtained for all experiments can be considered as very encouraging for both puff and continuous releases.

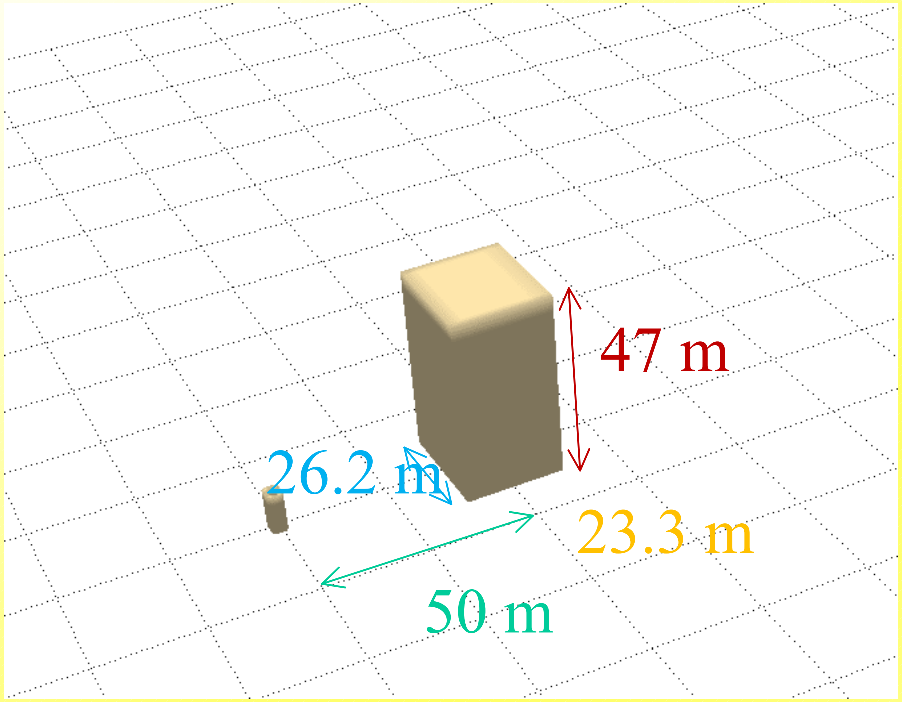
- They well agree with different versions of HEGADAS (Hanna and Chang, 2001), as well as CFD code FLACS (Hanna et al., 2004).

- Additional work, including more specific comparisons, is planned. This includes:
  - Use of all sonic anemometer data (7 masts) to reconstruct the 3D wind field and turbulence
  - Comparison of the 3D shape of the plume (height and width)
  - Cloud arrival time at the arcs

MERCURE and MSS simulation of dispersion in presence of obstacles

Building

- Xo = 50 m from release
- H = 47 m, Lx =23.3 m, Ly = 26.2 m



initial momentum vertical, w	= 1.14 m/s
emission height	= 10 m
initial density ratio (plume/air)	= 2.0
initial emission diameter	= 2.17 m
gas emission rate	= 10 kgs^{-1}

neutral stratification, logarithmic wind profile

2 flow regimes
- low wind at 10 m = 1.5 m/s
- higher wind at 10 m = 5 m/s

MERCURE - MSS

Mercure

domain 650 m x 550 m x 160 m

horizontal grid spacing is 0.7 m (near the release) up to 30 m

vertical grid spacing is 2 m (near ground) up to 10 m.

Swift and MicroSpray

domain 500 m x 200 m x 200 m

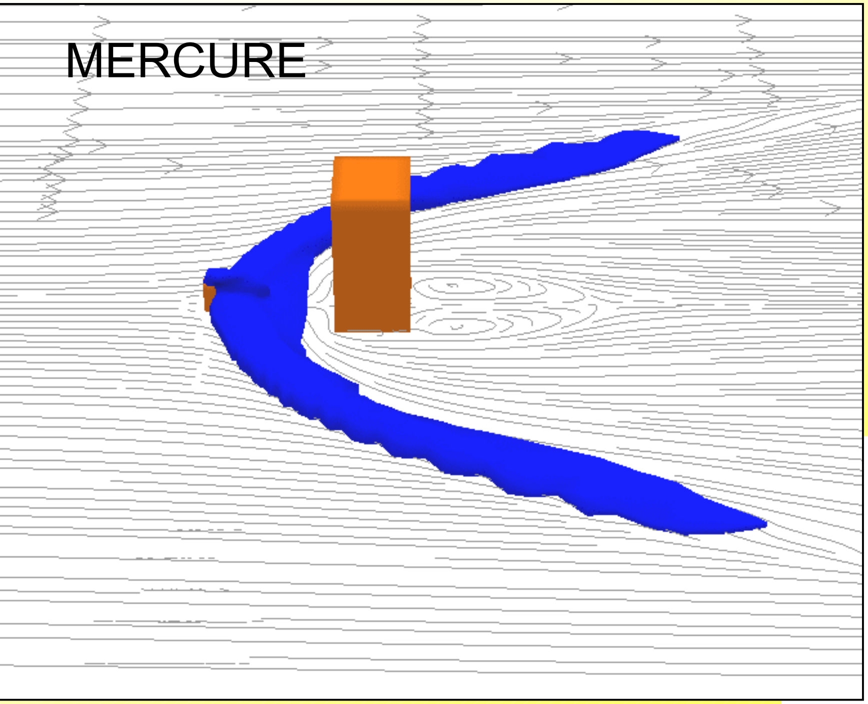
Swift

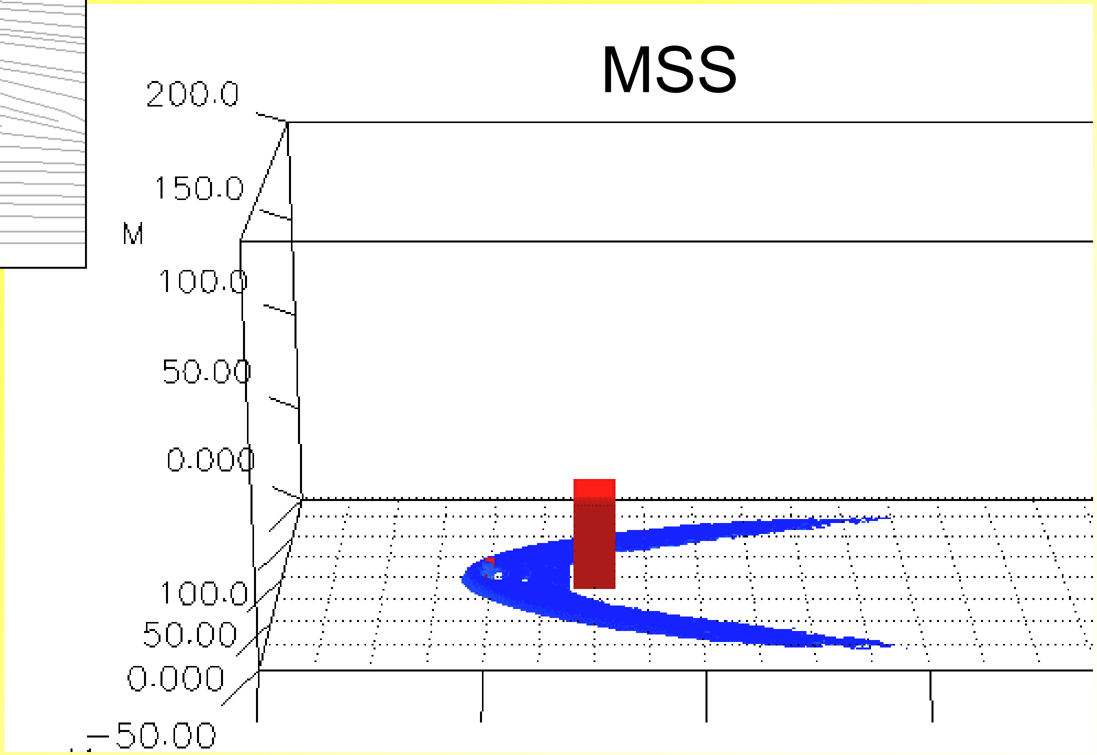
horizontal grid spacing is 1 m

vertical grid spacing is 0.5 m (near ground) up to 200 m

Wind(z=10m) = 1.5 m/s

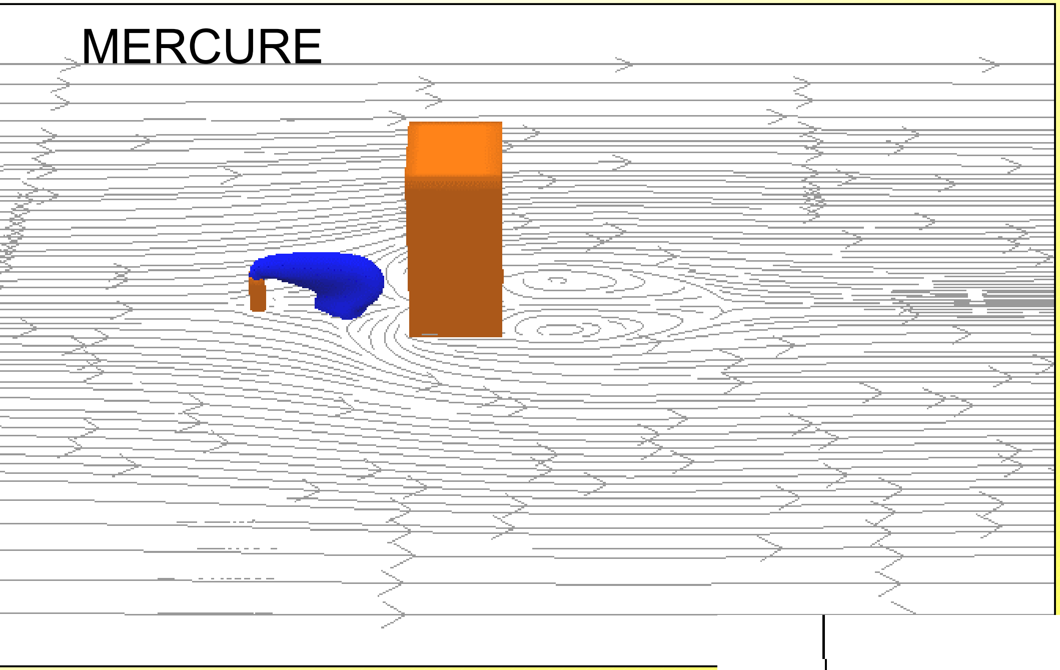
Iso-surface 0.01 kg/kg

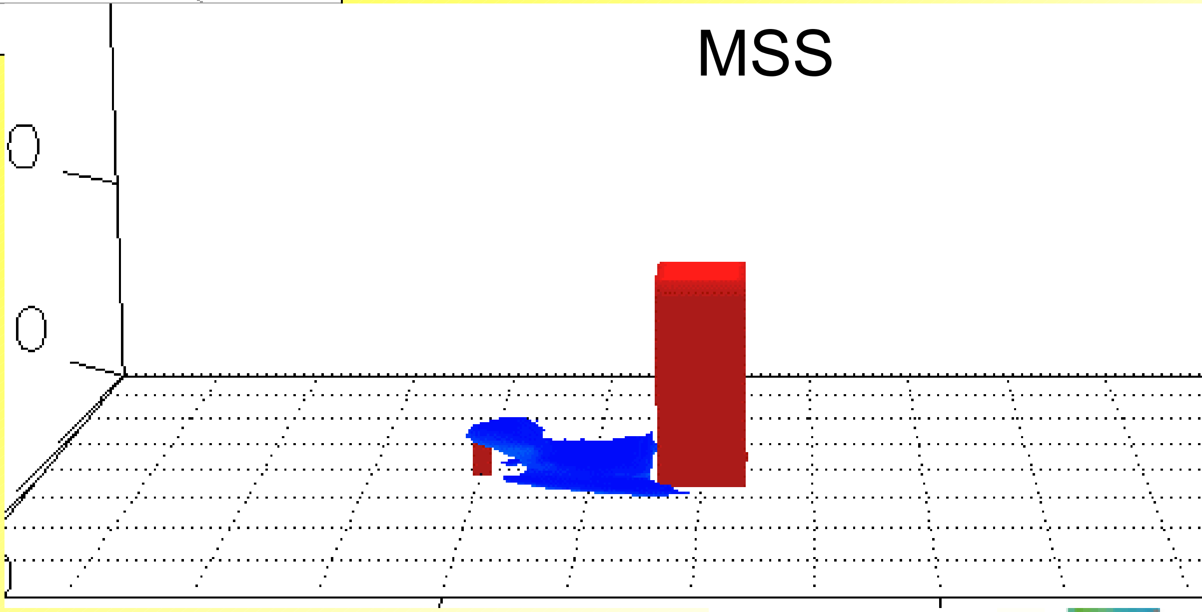




Wind(z=10m) = 5.0 m/s

Iso-surface 0.01 kg/kg

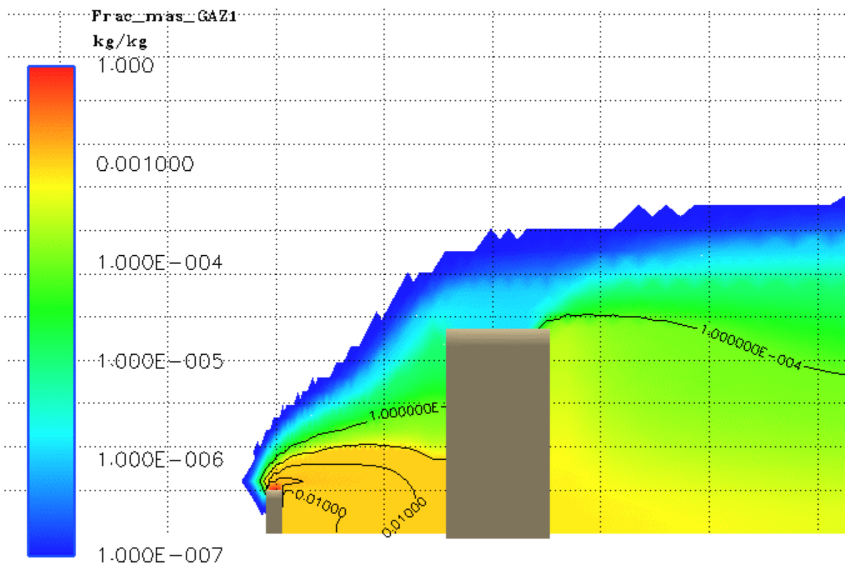




MERCURE

dense gas MRCR 12

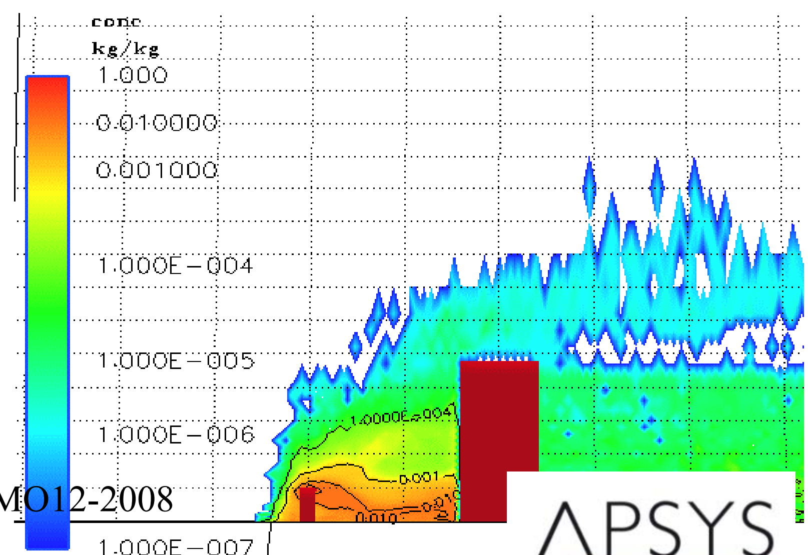
Vertical cut



Wind(z=10m) = 5.0 m/s

Vertical cut

dense gas MRCR 12 - MSS



MERCURE

CONCLUSIONS

A new version of the LPD model **MicroSpray,** devoted to simulate the dense gas dispersion in presence of obstacles, was validated by comparing its simulations with:

a real field accident (the Macdona railroad accident)

Kit Fox tracer experiments

and making an intercomparison between

MicroSpray and **CFD Mercure**

Results suggest that MicroSpray performs reliable simulations of dense gas dispersion

Thank you for the attention