Development of the micro-scale Lagrangian particle dispersion model MicroSpray for the simulation of two-phase releases

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- modified bouncing against obstacles and particle reflection at the domain bottom due to the cloud density

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- Subsequent entrainment will warm the cloud until it asymptotically reaches the ambient pressure.

Mass Conservations Equations

$$\frac{d}{dt}\left[\frac{\rho_p}{\rho_a}u_s b^2\right] = E u_s \tag{2}$$

Glendening, J.W., J.A. Businger, and R.J. Farber (1984)

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Anfossi et al., 2010 A new Lagrangian particle model for the simulation of dense gas dispersion. Atmospheric Environment 44, 753-762

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Drag term

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The coldness of the cloud is as important as the molecular weight of the contaminant in determining its density.

Homogeneous Equilibrium Assumption (Sykes et alii,1998)

$$m_{vc} = \frac{P_{cs}(T_p)M_c}{P_a M_v} \tag{6}$$

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Equation of state

$$\rho_p = \frac{\rho_a}{\alpha T_p + \gamma T_a} \tag{9}$$

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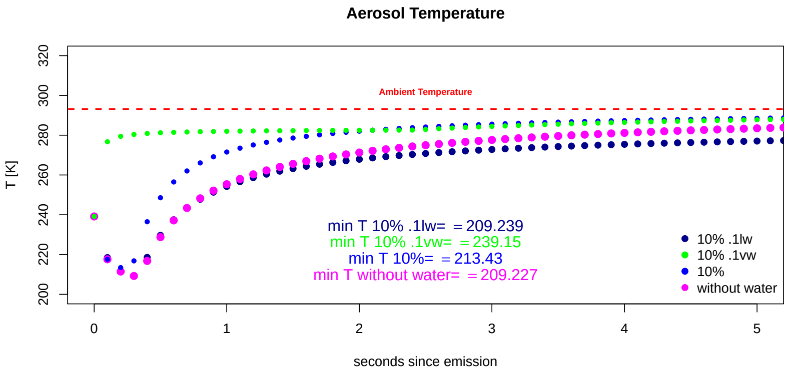
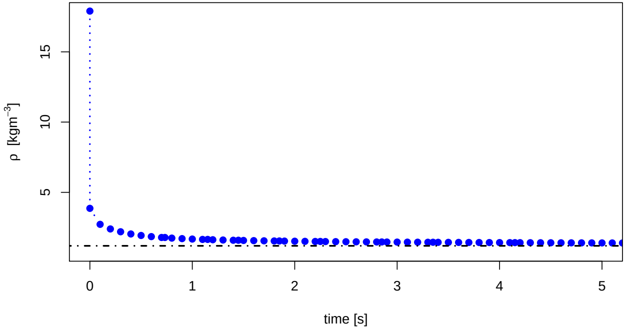
- *10 % .1lw*, a mixture of chlorine, 10% vapor and 80% liquid, and liquid water, 10%, is released in ambient air with relative humidity of the 10%.



The overall behavior of the system seems correct showing an initial loss of temperature due to the evaporation of the liquid part, this process seems to be reasonably balanced by the liquid water condensation. The model proved to be solid even in the extreme case of an initial condition of 10% liquid water inside the plume.

Density



In the very first instants of the simulation the density gradient is very steep and the initial density is very quickly lost, the loss is due to the fast vaporization of the liquids in the aerosols.

Plume spread on the ground

When a dense plume reaches the ground, its weight generates an horizontal momentum that tends to spread the plume.

The heavy gas induced *outflow velocity* depends on the bulk properties of the dense plume, i.e. it depends on the 3D density field and it is obviously not a characteristic of the single particle.

As long as the movement of each particle depends on the characteristics of the *ensemble* a hybrid Eulerian-Lagrangian algorithm is needed.

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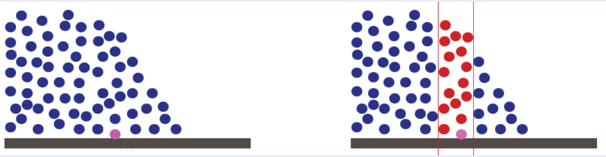
$$\begin{cases} U_{gs} = U_g sin\gamma \\ V_{gs} = U_g cos\gamma \end{cases} \qquad (11)$$

where γ is a random angle extracted from a uniform distribution

When a particle *reaches* the ground all the n_p particles belonging to the same column (on an Eulerian grid) are accounted for estimating the bulk properties of the plume.

Particle reflection on the ground



$$H_{bulk} = \frac{1}{n_p}\sum_{i=1}^{n_p} z_i \qquad \rho_{bulk} = \frac{1}{n_p}\sum_{i=1}^{n_p} \rho_i$$

Macdona chlorine railway accident, 28 June 2004

Railroad Accident Report NTSB/RAR-06/03

The comparisons presented here refer to Hanna (2007) report: *Comparisons of Six Models using Three Chlorine Release Scenarios (Festus, Macdona, Graniteville)*

Six widely-used hazardous gas models (SLAB, HGSYSTEM, ALOHA, SCIPUFF, SAFER/TRACE, PHAST) performances 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

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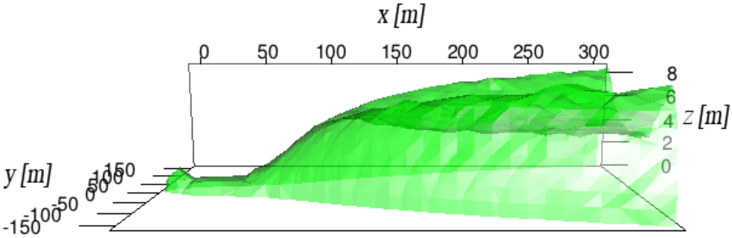
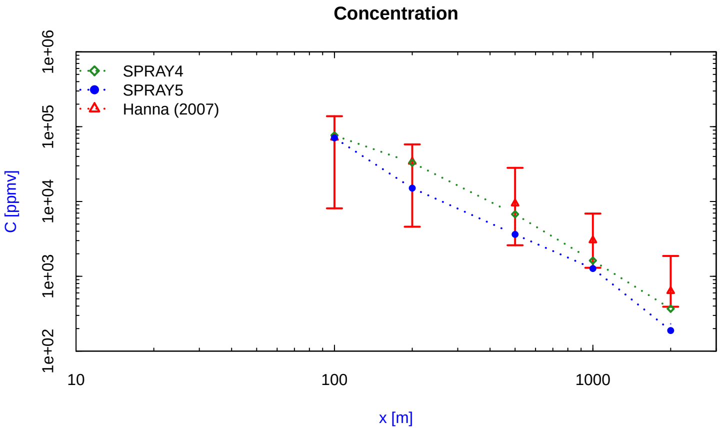
- downwind distances: 0.1, 0.2, 0.5, 1.0 and 2.0 km

2000 ppm Concentration Contour



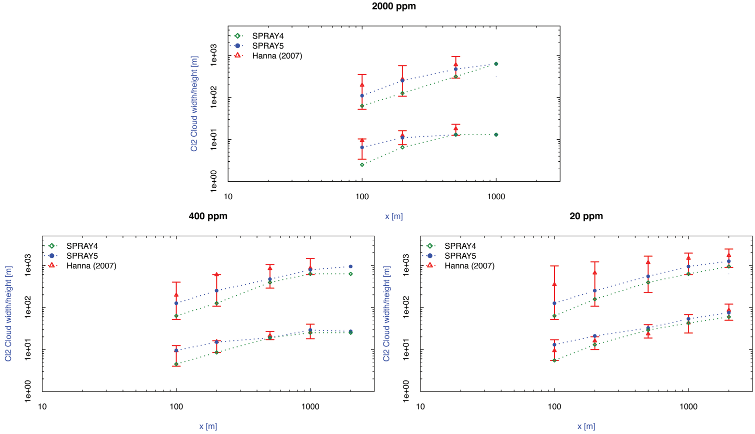
The 2000 ppm 3D contour plot gives an idea of the shape of the contaminant cloud. Up to $50\ m$ from the source the dynamic of the plume is dominated by the initial momentum while at farthest distances it is regulated by buoyancy. From $150\ m$ to $300\ m$ a lowering of the contour at the centre can be noticed, the dense cloud weight induces gravity spreading and radial outflow velocity increasing the contaminant concentration on the sides of the plume.

Chlorine concentration versus distance



Cl_2 maximum 10 minutes average concentration.

Chlorine cloud width and height at 20, 400 and 2000 ppm



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- emission model
- flashing
- rain out

Acknowledgements

The authors would like to explicitly remind that the distribution, maintenance and development of MicroSpray are carried out in collaboration with ARIA Technologies.

Thank you!

l.mortarini@isac.cnr.it