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DEVELOPMENT OF THE MICROSCALE LAGRANGIAN PARTICLE DISPERSION MODEL MICROSPray FOR THE SIMULATION OF TWO-PHASE RELEASES

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Abstract: A new version of the Lagrangian dispersion model MicroSpray was developed to simulate the dispersion of two-phase aerosol clouds. The model extends the algorithms developed to take into account the effects of dense gas dynamics recently developed for the code, allowing the simulation of gas-aerosol jets forming from accidental release of toxic industrial chemicals (TIC) stored in liquid phase in a pressurized vessel or pipe. The mixture of contaminant liquid and vapor is considered as a single material and each particle tracked by the model simulates the contaminant liquid and vapor, water liquid and vapor and dry air taking into account all the possible phase transformations and the related effects on the dynamics of the plume. A system of differential equations is solved to follow at the same time the dynamics and the thermodynamics of the plume to evaluate the liquid and vapor mass fractions after the initial flashing, taking into account the presence of water initially in the mixture or entrained from the wet ambient air. The state of the contaminant at each time step is determined assuming homogeneous thermodynamic equilibrium. The equation of energy conservation is rewritten to include the latent heats of the liquid contaminant and atmospheric water.

A sensitivity analysis showing the dependence of the model output on the time-step chosen and the influence of water vapor entrainment in the emission temperature drop has been performed. Further, to evaluate the MicroSpray ability to simulate the dispersion of two-phase releases of heavy gases, the model has been coupled with the diagnostic MicroSwift model, that provides the 3-D wind field in presence of obstacles and orography, and its performances compared in detail to a chlorine railway accident (Macdona). The simulations results, with and without the aerosol module, are presented and the differences are discussed.

Key words: Lagrangian models, two-phase releases, dense gases, toxic industrial chemicals, pollutant dispersion.

INTRODUCTION

Toxic industrial chemicals (TIC) are daily produced and transported. In case of accident their release and dispersion may be a severe threat to the population and consequently predicting the possible distribution of the pollutants may be helpful to decide safety measures to prevent dangerous situations. Hazardous substances are often stored in pressurized vessels where the contaminant is stored in its liquid phase. After a sudden rupture of the vessel the superheated liquid flashes producing a gas-aerosol mixture with temperature close to its boiling point (i.e. several degrees below the air temperature) where the liquid and vapour phase coexist. The cloud temperature and density are significantly different from the ambient ones, hence close to the source the emitted plume dispersion is strongly influenced by the thermodynamics of the liquid-phase transition and by the negative buoyancy due to its density. To study the dispersion of hazardous substances it is necessary to have a model that simultaneously takes into account phase transformations (of both the contaminant and of the water vapour entrained), density effect and the gravity spreading caused by the cloud weight.

Besides the ability of predicting the dynamics of two phase releases, the dispersion simulation of TIC releases in real case scenarios is complicated by the non-homogenous conditions created by the presence of buildings and obstacles and by complex orography. A fast, effective and reliable way to simulate these conditions is offered by Lagrangian Particle Models (LPDs). This approach is a compromise between the heavy computational demand of computational fluid dynamics models and the simplicity of integral models. Starting from the previous work of Anfossi et al. (2010), who studied the dispersion of heavy gases neglecting the thermodynamics, we present a new module of the Lagrangian Particle Model MicroSpray (Tinarelli et al., 2007) able to simulate the dispersion of hazardous releases of two-phases TIC jets.

MODEL PRESENTATION

Together with MicroSwift (Tinarelli et al., 2007), MicroSpray constitutes the MSS (Moussafir et al., 2004) model system. MicroSpray is a Lagrangian particle dispersion model based on a 3D form of the Langevin equation for the random velocity (Thomson, 1987) and is able to take into account the presence of obstacles and orography. The position of each particle is given by:

$$dx_i = (\bar{u}_{ai} + u'_i + u_{bi}) dt \quad (1)$$

where \bar{u}_{ai} is the mean wind velocity vector, u'_i is the turbulent velocity computed by a Langevin equation and u_{bi} is an additional velocity accounting for the buoyancy effects. The present version of the MicroSpray model is oriented to deal with dense gas dispersion in industrial sites and in the urban environments. The new module is able to deal with two-phase releases (vapour-liquid), aerosol evaporation and latent heat processes in the dispersing plume. In addition the model takes into account plumes without initial momentum and with initially arbitrarily oriented momentum (horizontal, vertical or oblique in any direction), positive or negative buoyancy, continuous and instantaneous emissions, time varying sources, elevated and ground level emissions, cloud spread at the ground due to gravity, bouncing against obstacles and particle reflection at the domain bottom in presence of a dense cloud. At present the flashing of the liquid is not accounted for and MicroSpray still needs a source emission model (Britter et al., 2011) as input. Immediately after the flashing the release is mostly vapor by volume and liquid by mass, therefore dealing with the physics of the aerosols implies the introduction of the liquid phase of the contaminant and, if necessary, of the water vapor entrained. The entrainment of ambient air produces a decreasing of the partial pressure and hence a cooling of the mixture below its boiling point and the condensation of water. The total mass of each particle needs to be split in five different contributions:

$$m_{vc} + m_{ic} + m_{vw} + m_{iw} + m_{da} = 1 \quad (2)$$

the various term being the mass fraction, respectively: m_{vc} of the contaminant in vapor phase, m_{ic} of the contaminant in liquid phase, m_{vw} of the water vapor, m_{iw} of water in liquid phase and m_{da} of the dry air mass. Glendening et al. (1984) mass conservation equation needs to be written for each specie, contaminant, water and dry air:

contaminant mass conservation:
$$\frac{d}{dt} \left[\frac{\rho_p}{\rho_a} (m_{vc} + m_{ic}) u_s b^2 \right] = 0 \quad (3)$$

water mass conservation:
$$\frac{d}{dt} \left[\frac{\rho_p}{\rho_a} (m_{vw} + m_{iw}) u_s b^2 \right] = m E u_s \quad (4)$$

dry air mass conservation:
$$\frac{d}{dt} \left[\frac{\rho_p}{\rho_a} m_{da} u_s b^2 \right] = (1 - m) E u_s \quad (5)$$

These equations are coupled with three momenta conservation equations and with the energy conservation equation (enthalpy balance).

vertical momentum conservation:
$$\frac{d}{dt} \left[\frac{\rho_p}{\rho_a} u_s w_p b^2 \right] = g \frac{\rho_a - \rho_p}{\rho_a} b^2 u_s \quad (6)$$

x horizontal momentum conservation:
$$\frac{d}{dt} \left[\frac{\rho_p}{\rho_a} u_s b^2 u_p \right] = E u_s u_a - C_g u_p b (u_a - u_p)^2 \quad (7)$$

y horizontal momentum conservation:
$$\frac{d}{dt} \left[\frac{\rho_p}{\rho_a} u_s b^2 v_p \right] = E u_s v_a - C_g v_p b (u_a - v_p)^2 \quad (8)$$

energy conservation:
$$\frac{d}{dt} \left(\frac{\rho_p}{\rho_a} u_s b^2 C_p T_p \right) = \frac{d}{dt} \left[\frac{\rho_p}{\rho_a} u_s b^2 (m_{ic} L_c + m_{iw} L_w) \right] + C_a T_a E u_s \quad (9)$$

Regarding the momenta conservations equations: ρ_p is the plume density, ρ_a is the air density, u_s is the module of the particle velocity, (u_p, v_p, w_p) , b is the plume instantaneous radius, g is the gravity acceleration, E is the entrainment, u_a and v_a are the horizontal component of the ambient velocity and T_p is the plume temperature, the liquid aerosol and vapor are taken to be in thermodynamic equilibrium, therefore a single temperature characterizes the cloud (homogeneous equilibrium model). Equations 7 and 8 were modified introducing a negative term representing the drag force which strongly influence the dynamics of turbulent jets close to the source. In the simulations presented in this paper the drag coefficient, C_g , has been set to 0.1.

Regarding the energy conservation: C_p is the mixture specific heat, C_a is the ambient air specific heat, L_c and L_w are the latent heat of evaporation for contaminant and water and T_p, T_a are the plume and air temperature. To solve the new system of equations the equation of state for vapour mixtures has to be considered (Ermak, 1990):

$$\rho_p = \frac{\rho_a T_a}{\alpha T_p + \gamma T_a} \quad (11)$$

α and γ being two parameters depending on the mass fractions and the molecular weight of the mixture.

The homogeneous equilibrium assumption implies that for each component the vapour pressure is equal to the saturation pressure, P_{cs} , and that the vapour and liquid mass fractions are given by (Sykes et al., 1998):

$$m_{vc} = \frac{P_{cs}(T_p) M_c}{P_a M_v} \quad (12)$$

$$m_{vw} = \frac{P_{ws}(T_p) M_w}{P_a M_v} \quad (13)$$

where M_c and M_w are the molecular weights of the contaminant and of the water and M_v is the molecular weight of the mixture:

$$M_v^{-1} = m_{vc} M_{vc}^{-1} + m_{vw} M_{vw}^{-1} + m_{da} M_{da}^{-1} \quad (14)$$

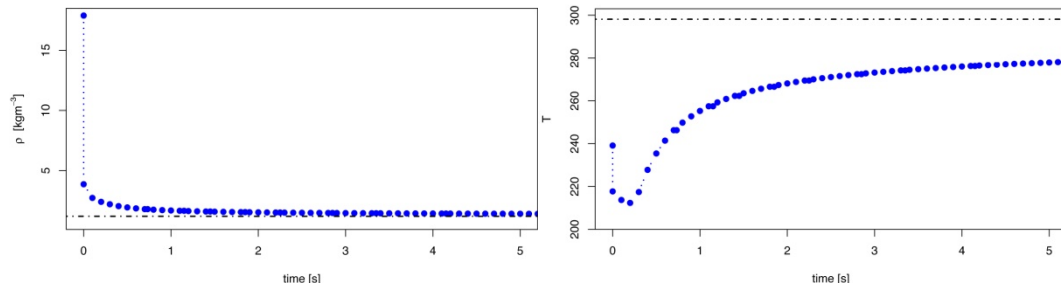


Figure 11. Density (left) and temperature (right) evolutions of a single Lagrangian particle (blue dots). The dot-dashed line refers to the ambient value at the source height.

MODEL RESULTS

A typical real case scenario for two-phase releases is the sudden venting of a superheated liquid from a pressured vessel. Therefore, we chose to test the performances of the new MicroSpray module with the Macdona chlorine railway accident (Hanna, 2007). The simulations were run using MicroSpray 5.2 under the same input provided in Hanna (2007). A computational domain of 2200 m x 1400 m x 1000 m was considered. MicroSwift had a horizontal grid spacing of 10 m and a stretched grid in the vertical. One thousands particles were released per second from a 1-m-high source with an initial diameter of 0.561 m and exit speed of 100 ms⁻¹. The rapid release was treated as an adiabatic process with the contaminant in liquid and vapor phases at a temperature equal to the chlorine normal boiling point, 239.15 K. Relative humidity was 100% and the emission was initially 80% liquid and 20% vapor, no water was considered at the source. The emission lasted 136 s, whereas the dispersion simulation lasted 30 min.

Figure 1 shows the behaviour of temperature and density of a single particle of the contaminant cloud in the first instants. As for the density it can be noticed that in the very first instants of the simulation the gradient is very steep and the initial density is very quickly lost, the density loss is due to the fast vaporization of the liquids in the aerosols. Regarding the temperature, as ambient air is entrained into the cloud, the partial pressure of contaminant decreases, the aerosol vaporizes and cools down the plume. The significant reduction of the initial temperature is partially balanced by the condensation of water vapour. Later, when the entire contaminant mass is vaporized, more and more ambient air is entrained and the cloud temperature increases until it reaches the ambient temperature.

Figure 2 shows the 2000 ppm 3D contour plot and gives an idea of the shape of the contaminant cloud. It is clear that 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.

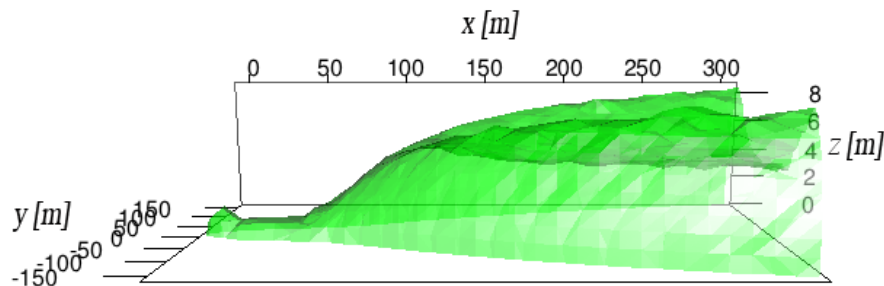


Figure 12. 2000 ppm 3D contour plot, the concentration is averaged on the first 10 minutes of the release.

In order to have a quantitative comparison we also compared the MicroSpray results with six dispersion models presented in Hanna (2007). For this purpose, we computed: the maximum model-simulated 10 min average chlorine concentration at four down-wind distances (100, 200, 500, 1000 and 2000 m), plume widths and plume heights in correspondence to the model-simulated concentration of 2000, 400, and 20 ppm at the same distances. The results are shown in figure 3. The vertical bars indicate the variability (min, max) of the six models and the triangles locate the median of these models. As for the concentration MicroSpray results are inside the models' variability except for the last point that shows a lower concentration. The concentration width and height comparisons show that MicroSpray results are always well within the prescribed range, the simulated plume is narrower almost of the same height than the median of the other models ensemble. Unfortunately, the lack of experimental data close to the source makes very difficult to test the two-phase module in the near field. However the accuracy of the new MicroSpray module is comparable with the one of the other models.

If compared with its older version (Anfossi et al., 2010), where no liquid phase was modeled, temperature and pressure played an identical role and the where the initial density of the plume was derived from Hanna (2007, Table 2, initial values suggested for modelers), the new MicroSpray produces lower concentrations at 200 m and 500 m, but it better reproduces the

maximum widths and heights of the different concentration profiles, hence the dilution of the plume and the concentration contours' distribution are more similar to the one evaluated by the other six models.

It might be stressed that the introduction of the two-phase processes fairly enlarges the capabilities of MicroSpray. The inclusion of the thermodynamics of aerosols draws the model closer to the source, taking into account jet releases well before they reach an equilibrium with the ambient velocity. The lack of an emission model (Britter et al., 2011) might be reckoned as a shortcoming. However, any initial condition in accidental TIC releases often needs "fit-for-purpose" approaches (type of contaminant, geometry, thermodynamic state, type of rupture). Since it is very unlikely to have general guidance, each single case has to be separately considered.

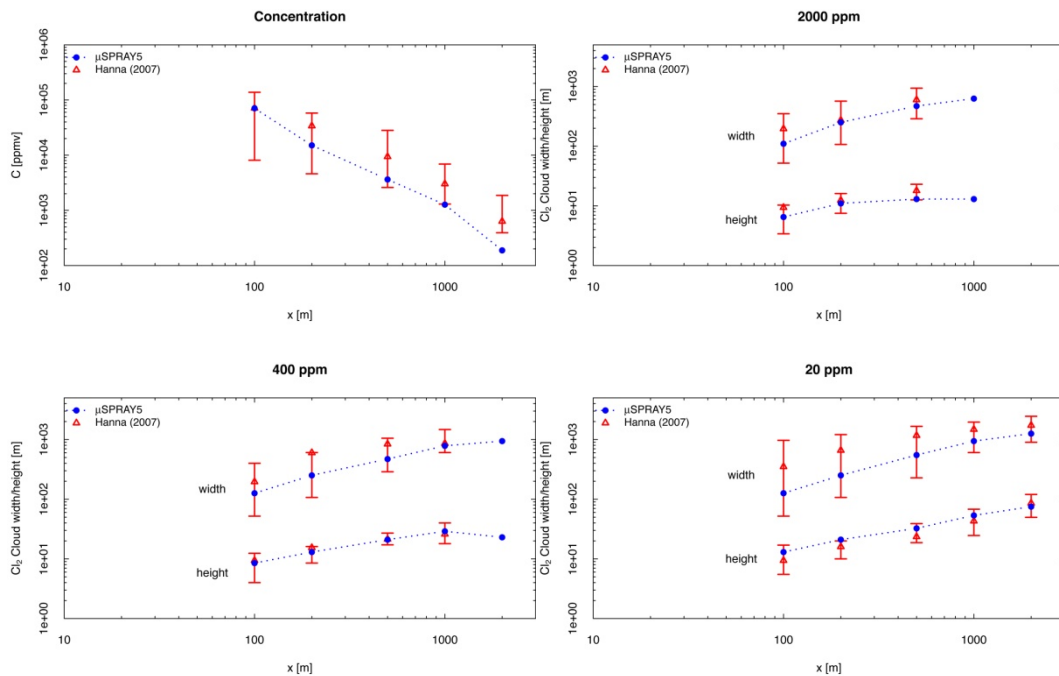


Figure 3. Maccona accident simulations inter-comparison. Full circles and dotted line (blue): MicroSpray5 results; vertical bars (red): six models (Hanna, 2007) ensemble variability (min, max); empty triangles: median of the six models. (top left): maximum 10 min average Cl_2 concentration versus downwind distance. (top right, bottom left and bottom right), Cl_2 cloud width and height corresponding to model-simulated concentration of 2000 ppm, 400 ppm and 20 ppm.

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