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# DEVELOPMENT AND APPLICATION OF THE MICROSCALE LAGRANGIAN PARTICLE DISPERSION MODEL MICROSPRAY FOR THE SIMULATION OF ACCIDENTAL HYDROGEN RELEASES.

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**Abstract**: A new version of the Lagrangian dispersion model MicroSpray was developed to simulate the dispersion of light gas emitted at high speed. The model was used and tested in the frame of the BioH2Power Project to describe the accidental release of hydrogen gas at supersonic emission speed. A preliminary analysis of the performance of the model is here proposed versus the data observed during an experimental field campaign carried out in Tuscany (Italy).

***Key words:*** *Lagrangian dispersion model, light gases, accidental releases, jets, experimental campaign.*

## INTRODUCTION

The accidental release and dispersion of hazardous, toxic or explosive gases may cause severe problems to the population and the environment of the area where such materials are handled. These hazardous clouds may be emitted initially less dense than the ambient air and often, because of high storage pressure, have a very high initial speed. In particular, hydrogen is stored in cylinders at very high pressures and it is highly flammable, thus its transport and settlement in plant sites present the risks of accidental high-pressure releases and explosions. It is important to have a model able to simulate and predict an accidental dispersion of the gas and to correctly estimate the area possibly affected by critical concentration levels, even leading to explosions, where the population might be injured. The model needs to be both accurate, since releases generally occur in complex terrain and in presence of obstacles, and fast running, since an emergency response for the dispersion scenario is expected in very short times.

In the frame of the BioH2Power Project, the implementation of such requirements was pursued developing a new version of the Lagrangian model MicroSpray, apt at simulating high pressure and high speed releases of light gases. The model was tested in the case of an experimental campaign, during which six hydrogen releases from a cylinder (pressure of 1 MPa and exit velocity of about 1900 $ms^{-1}$) were measured and analysed. The results from the numerical simulations of the experimental trials are quite encouraging and show that MicroSpray is performing well even in such extreme condition. The model is able to reproduce the gas motion and to give a reasonable concentration estimation, also with a supersonic jet of a buoyant gas in an environment where the time and space scales belong to the lower range of the microscale (s and cm), and with all the uncertainties related to the experimental conditions and affecting the optimal comparison between predictions and observations. This research supports the evaluation of the technical reliability and safety, and the social acceptability, of different and alternative unit plants for the production of hydrogen from biogas.

## OUTLINE OF THE NEWLY DEVELOPED VERSION OF MSS MODELLING SYSTEM

MicroSpray is part of the model system MSS (Moussafir *et al.*, 2004; Tinarelli *et al.*, 2007) that includes MicroSwift and MicroSpray. MicroSwift is an analytically modified mass consistent interpolator over complex terrain. Given topography, meteorological data, buildings and obstacles, a mass consistent 3-D wind field is generated. It is also able to derive diagnostic turbulence parameters to be used by MicroSpray inside the flow zones modified by obstacles. MicroSPRAY is a Lagrangian Particle Dispersion Model (LPDM) able to take into account the presence of obstacles. It directly derives from SPRAY code (Anfossi *et al.*, 1998; Tinarelli *et al.*, 1994 and 2000; Ferrero *et al.*, 2001; Carvalho *et al.*, 2002; Trini Castelli *et al.*, 2003) and it is based on a 3-D form of the stochastic Langevin equation for the random velocity.

In MicroSpray the turbulent velocity and the displacement of each particle are given by the following equations:

$$du_i' = a_i(\boldsymbol{x},\boldsymbol{u},t)dt + b_{ij}(\boldsymbol{x},\boldsymbol{u},t)dW_j(t) \qquad (1)$$

$$dx_i = \left(\overline{u}_{ai} + u_i' + u_{bi}\right)dt \qquad (2)$$

where $i,j$=1,2,3 , $\overline{u}_{ai}$ is the mean wind velocity vector, $\boldsymbol{u}$ is the Lagrangian velocity vector, $u_{bi}$ is an additional velocity accounting for the buoyancy effects, $a_i(\boldsymbol{x},\boldsymbol{u},t)$ is a deterministic term and $b_{ij}(\boldsymbol{x},\boldsymbol{u},t)$ is a stochastic term and the quantity $dW_j(t)$ is the incremental Wiener process. The deterministic coefficient depends on the Eulerian probability density function (PDF) of the turbulent velocity and is determined from the Fokker-Planck equation. The stochastic term is obtained from the Lagrangian structure function and is related to the Kolmogorov constant, $C_0$, for the inertial subrange. In the standard MicroSpray version, the rise of hot plumes if any, is accounted for in a simplified way (Anfossi *et al.*, 1993). Input data, such as wind velocities, standard deviation and Lagrangian time scales are assigned to each particle, at each time step, through a 4-D interpolation linear in space, among the eight closest Eulerian grid points, and in time, between two subsequent input meteorological files.

The new version of MicroSpray model is especially oriented to deal with light, or dense, gas dispersion in urban environment and industrial sites. It accounts for the following aspects: plume without initial momentum and with initially arbitrary oriented momentum, in any direction; positive or negative buoyancy; elevated and ground level emissions; instantaneous and continuous emissions; particle reflection at the domain bottom. In this work we focus our attention on the light emissions. At present, no source emission modules, treating the phase changes liquid-vapour that may occur at the source, are included.

In the so-called 'single-particle' Lagrangian models each particle trajectory is independent on the behaviour of the other cloud particles. Here we propose a hybrid approach that takes into account the characteristics of the 'ensemble' of particles, so that it depends on how density varies in 3D and requires all the particles positions to be considered together.
To deal with the first plume phase, in which the emission height and direction may be variable, five governing conservation equations of mass, energy, vertical momentum and two horizontal momenta are integrated for each particle at each time step, in addition to the standard calculations (Anfossi *et al.*, 2010):

$$\frac{d}{dt}\left[\frac{\rho_p}{\rho_a} u_s b^2\right] = E u_s \quad (3)$$

$$\frac{d}{dt}\left[u_s b^2 B\right] = -\frac{\rho_p}{\rho_a} N^2 u_s w_p b^2 \quad (4)$$

$$\frac{d}{dt}\left[\frac{\rho_p}{\rho_a} u_s w_p b^2\right] = B b^2 u_s \quad (5)$$

$$\frac{d}{dt}\left[\frac{\rho_p}{\rho_a} u_s b^2 u_p\right] = E u_s u_a \ , \qquad \frac{d}{dt}\left[\frac{\rho_p}{\rho_a} u_s b^2 v_p\right] = E u_s v_a \quad (6)$$

The variables appearing in the equations are defined as:

$$u_s = \sqrt{u_p^{\ 2} + v_p^{\ 2} + w_p^{\ 2}} \ , \quad u_e = (\alpha_1 u_s + \alpha_2 U_a), \quad B = g(\rho_a - \rho_p)/\rho_a \ , \quad E = 2bu_e$$

where: $a, p$ refer to air and plume, respectively, $b$ is the plume radius, $B$ is the buoyancy, $E$ represents the entrainment rate, $U_a$ is the wind velocity and $u_e$ is the entrainment velocity, $\alpha_1$ and $\alpha_2$ are the entrainment constants and ρ is the density; $u_p$, $v_p$ and $w_p$ are the particle velocity components, $u_a$ and $v_a$ are the horizontal components of the wind velocity, $N^2$ is the Brunt-Vaisala frequency. The first three equations (3-5) were derived by Hurley and Manins (1995) starting from Glendening *et al.* (1984) and previously proposed by Hurley (2005). The two remaining equations (6) were proposed by Anfossi *et al.* (2008), following the same procedure as in Hurley and Manins (1995).

At the emission, a normally distributed buoyancy flux is assigned to each particle, fixing the mean value equal to the mean buoyancy flux $B$ and the standard deviation equal to $B/3$. All these equations are solved for each particle, at each time step, provided the density of the particle is lighter than that of the ambient air. During the non-neutral phase the particle equation for the vertical component reads (see eq. 2):

$$dz = \left(\overline{w_a} + w_i' + w_p\right)dt \quad (7)$$

Afterwards, the particle continues its motion as a neutral particle, i.e. $w_p$ in the above equation is set equal to zero.

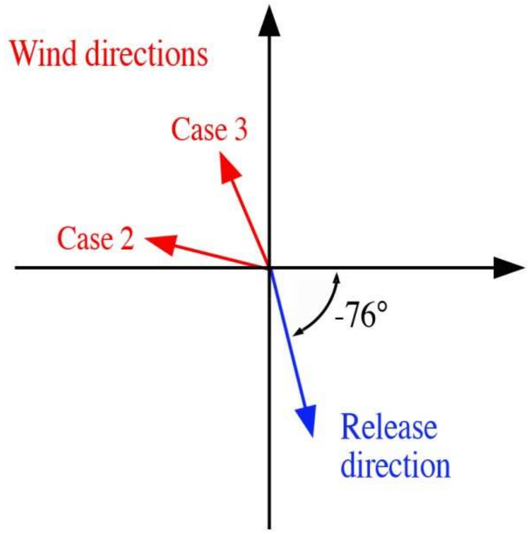
**DESCRIPTION OF THE PISA EXPERIMENT**
The Hydrogen Pipe Break Test (HPBT) experimental apparatus was installed within the Laboratory "Scalbatraio" of the University of Pisa (Mattei *et al.*, 2009), in an open field in Tuscany (Italy). This apparatus was used to investigate the behaviour of $H_2$ leakages from pipelines; it was able to simulate a real, low pressure $H_2$ release into free air. The pressure system was designed to have a maximum working pressure of 1 MPa. Discharge orifices of varying diameters and discharge pressure were changed to study different accidental conditions. The supply system used (four storage tanks of 3 $m^3$ each) was set in such way that with the largest orifice (1.1 $10^{-2}$ m diameter) the maximum discharge pressure could be maintained for about one minute before the pressure began to drop below 0.7 MPa. At lower pressure the jet length became too small for the task of the research, and the recharge of experimental apparatus was too expensive to take this action. All the releases were directed horizontally, 0.9 m above the test ground, with a slight upwards inclination of 4°, due to an installation problem.

During the experimental campaign a total of 22 tests were performed, six of them with hydrogen: five of these last were suitable for the comparison with the model simulations. Different setups of the experiment were considered, varying the hole diameter (D=0.25 $10^{-2}$ m; 0.5 $10^{-2}$ m; 1.1 $10^{-2}$ m) and the internal pressure (P=0.2 MPa; 0.5 MPa; 1 MPa). Here we discuss two of these tests, from the second (Case 2) and the third (Case 3) releases, both performed with D=1.1 $10^{-2}$ m and P=1 MPa, because they represent an interesting benchmark for testing the MSS numerical simulations. In the experiments the following data were acquired: oxygen concentration, internal pressure, internal temperature, wind speed and direction. The pressure and the temperature of hydrogen close to the release nozzle and in the storage tanks were recorded during each test in order to control the release. The air temperature, wind intensity and direction were measured continuously near the release point using a sonic anemometer and a thermocouple. Since the available hydrogen sensors do not work properly in free air, hydrogen concentrations were derived at eight different points from measurements of the oxygen concentration, under the assumption that any decrease in the concentration of oxygen was caused by the displacement of oxygen induced by the hydrogen gas plume. The eight measurements points were chosen in a spatial configuration allowing to study the jet shape and wind influence, five along the release direction, two displaced in the cross horizontal direction and one displaced in the vertical.

Table 1 summarises the meteorological parameters evaluated from the wind data, in Figure 1 (left) the release and wind angles for both cases are depicted and in Table 2 the position of the five samplers along the release direction is given.

Table 1. Meteorological parameters evaluated from the wind data

| Case | Wind Direction [degree] | Wind speed [$ms^{-1}$] | $u_*$ [$ms^{-1}$] | $z_0$ [m] | $\sigma_u$ [$ms^{-1}$] | $\sigma_v$ [$ms^{-1}$] | $\sigma_w$ [$ms^{-1}$] |
|---|---|---|---|---|---|---|---|
| 2 | 114 | 0.96 | 0.13 | 0.052 | 0.30 | 0.57 | 0.11 |
| 3 | 157 | 1.61 | 0.10 | 0.016 | 0.66 | 0.29 | 0.09 |



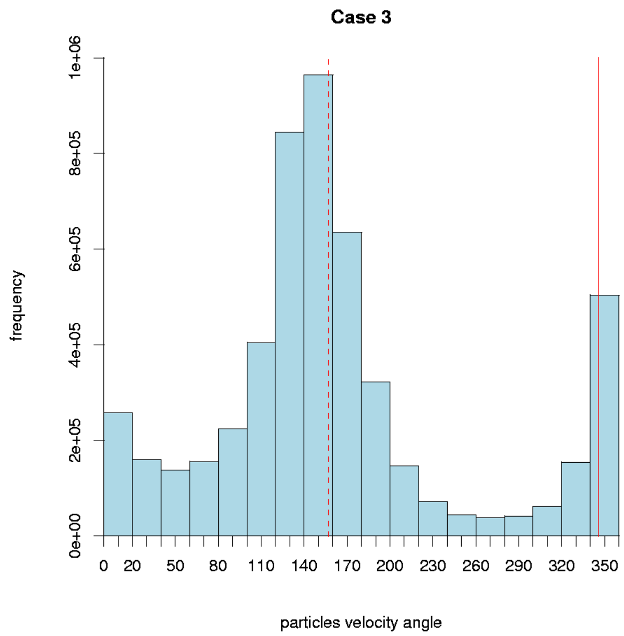




Figure 1. Wind and emission directions in the meteorological system during the two releases (left) and histogram of the absolute frequency of occurrences for the particle velocity angles in Case 3 (right).

Table 2. Locations of the five probes displaced along the release direction as distance from the source.

| **Probe code** | | **S1** | **S2** | **S3** | **S4** | **S5** |
|---|---|---|---|---|---|---|
| **Distance in *x* from the source (*y*=*z*=0) [cm]** | *Case 2* | 14 | 52 | 92 | 127 | 198 |
| | *Case 3* | 62 | 93 | 123 | 200 | 306 |

**RESULTS AND DISCUSSION**

Cases 2 and 3 represent interesting case studies, since the wind direction is almost or orthogonal or opposite to the jet exit direction and they give the chance to verify the capability of the model in correctly reproducing the strong deviation of the plume with respect to its initial exit direction. In Figure 1 (right) a distribution frequency of the angles associated to the velocity directions of the particles is plotted in a histogram for Case 3. Two peaks occur in the distribution, in proximity to the exit velocity direction of the gas jet (solid red line) and to the wind direction (dashed red line). The two directions are calculated in the meteorological reference system. We evaluated that the puff of particles clusters around the jet direction, 346 deg, close to the emission, roughly within the first 2 m height above the source and in the first 3 m far from the source, then it definitely takes the wind direction. The dynamics of the interaction between the plume and the ambient wind is clearly visible also in Figure 2, where a horizontal (left) and vertical (right) projection of the plume is plotted for the Case 2.

It is possible to appreciate the deviation of the plume from its exit direction due to the effect of the wind on it, confirming that the model is able to describe such short-time evolution of the plume dispersion. We notice that even releasing a large number of model particles ($4.5\ 10^6$ in this case), very few of them reach the farthest probes, due to the rotation of the plume induced by the wind and the buoyancy. Considering also the relatively small volume around the probe where the particles are counted to compute the concentration, it is clear that when none among the few particles in that part of the domain is entering this discrete volume, the prediction will give a zero value for the concentration. This would result in a 'bad' performance of the model versus a non-zero measured value, even if this is very small and can be affected by large errors. This aspect is highlighted also in Figure 3, where the ratios between the predicted and measured concentrations are plotted for each sampler as a function of the sampling box. On the *x* axis the dimension of the vertical size *dz* of the box is reported, changing from 1 to 8 cm and determining the horizontal dimensions as *dx=dy=2.5 dz*

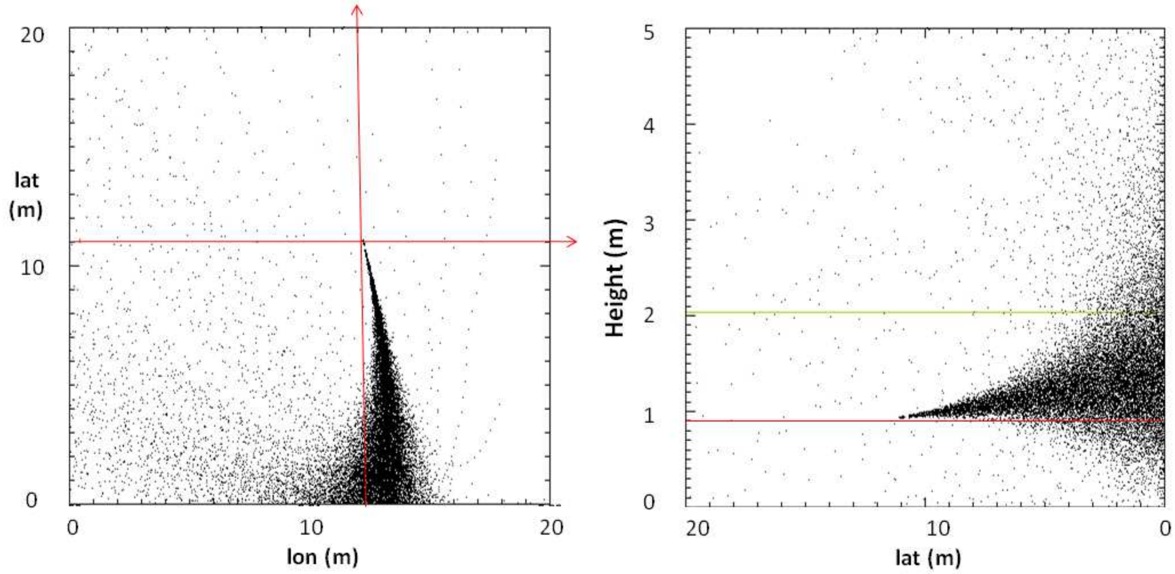



Figure 2. Case 2. Horizontal (left) and vertical (right) projection of the plume of particles in the simulation coordinate system.

The concentrations *C* at the five considered samplers (Table 1) were firstly calculated in a standard way (Figure 3), counting the number of particles in each grid cell and accumulating their masses *M*: $C(i,j,k) = M(i,j,k)/dxdydz$ .

Then, to account for the high emission speed, the contribution of each particle mass was weighted on the total time that the particle spends inside the cell during the integration time step *dt*, considering that the dominating velocity component is along the release direction, here $u_p$: $C(i,j,k) = \left(M(i,j,k)/dxdydz\right)u_p dt/dx$ .

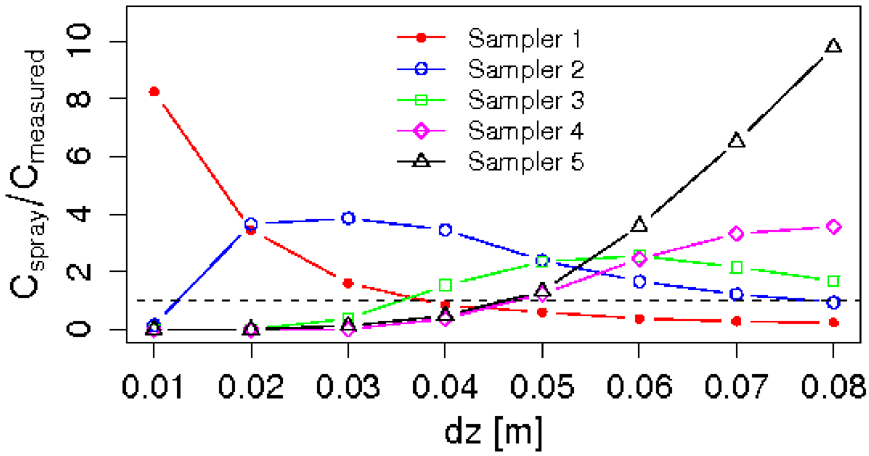



Figure 3. Case 2. Ratio between the predicted and observed concentrations at the sensors as a function of the dimension of the sampling box for the calculation

We notice that in the standard case the sensitivity to the sampling box is larger for the closest (S1) and farthest (S5) samplers. The box dimension providing the best agreement at the different samplers is given in Table 3, but in general *dz* ~ 4 cm gives the best results, while smaller(larger) dimensions bring to an under(over) estimation of the observed data. An over-estimation is almost always occurring at around 0.5 metres from the emission point, where sampler S2 is placed. In S2 *Ccal~Cobs* is obtained with the largest size of the sampling box. This overestimation has been found in all the cases and can be related to an erroneous determination of the emission vertical angle, combined with the probably critical distance of S2 sampler, still very close to the emission point but already sensitive to the spread of the plume. With supersonic jets a small uncertainty on this angle can produce large variation in the particles velocity.

Table 3. Sampling box dimensions giving the best agreement *Ccal* vs *Cobs* at the samplers for the standard calculation

| **Probe code** | **S1** | **S2** | **S3** | **S4** | **S5** |
|---|---|---|---|---|---|
| **Sampling box vertical dimension for which *Ccal/Cobs*=1 (cm)** | 4 | 8 | ~3.5 | ~4.5 | ~4.5 |
| **Sampling box volume for which *Ccal/Cobs*=1 ($m^3$)** | 0.4 | 3.2 | ~0.27 | ~0.57 | 0.57 |

When instead the concentrations are weighted on the 'flytime' of the particles, the sensitivity to the sampling box dimension is much less enhanced but the calculated concentrations drop to small values, mainly due to the very small time step used, $dt=10^{-4}$ s, which is needed to properly describe the fast evolution of the plume in such high-speed conditions. Therefore, a proper estimation of the predicted concentrations is a critical issue that needs deeper investigation.

The discrepancies between predicted and observed concentrations might be also related to the fact that the hydrogen measurement is an indirect one, since it is derived by the direct measurement of oxygen, as previously explained. This approach might lead to an underestimation of the actual concentration of hydrogen in the air. All these aspects are under investigation and further simulations are run, as discussed in the following Conclusions.

## CONCLUSIONS

The results from the numerical simulations of the Pisa experimental trials are quite encouraging and show that MicroSpray is performing rather well even in such extreme condition. In fact, also with a supersonic jet of a buoyant gas in an environment where the time and space scales belong to the lower range of the microscale, since we are dealing with seconds and centimetres, the model is able to reproduce the particles' motion and to give a reasonable concentration estimation.

It is also important to interpret the MicroSpray results in the light of the peculiarities of the experimental measurements. During the data analysis and the numerical simulations several issues were raised, related to the experimental conditions and affecting the optimal comparison between predictions and observations: the uncertainty in the emission angle with respect to the anemometer position; the strong fluctuations of the sensor position; the crucial dependence of the particles' dispersion on the initial conditions, related to the small scale and the velocity of the release.

These aspects suggest to perform further numerical simulations, varying the initial and boundary conditions in the model in order to investigate the effect of the input data uncertainty on the model performance and to gather useful information about the variability of the observed data, estimating their uncertainty.

Further modifications of the conservation equations for the plume are under investigation, in order to describe the transition from momentum-controlled jet to buoyancy-controlled jet with an approach that better details the physics of this process.

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