# MICROSPRAY SIMULATION OF DENSE GAS DISPERSION IN COMPLEX TERRAIN

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**Abstract**: An extended validation of the new Lagrangian particle model MicroSpray version for dense gas simulation is proposed. MicroSpray simulates the dense gas dispersion in situations characterized by the presence of buildings, other obstacles, complex terrain, and possible occurrence of low wind speed conditions. Its performances are compared to a chlorine railway accident (Macdona), to a field experiment (Kit Fox) and to an atmospheric CFD model.

***Key words:*** *dense gas dispersion, Lagrangian particle model, CFD, obstacles.*

## 1. INTRODUCTION

Accidental release and dispersion of hazardous gases and vapours may cause severe problems to the populations living adjacent to industries and storage areas, where such materials are handled. Consequently, understanding the possible distribution of the hazardous substances is important for the evaluation of the adequacy of safety measures to both prevent accidents and mitigate their effects. The simulation of dense gas dispersion for risk analysis purposes in real terrain poses specific difficulties related to complex terrain, presence of buildings and other obstacles.

In the present paper we present an updated version of the Lagrangian particle dispersion model MicroSpray, that was recently adapted to study dense gas dispersion (Anfossi et al., in press). This new version specifically accounts for the interaction of the dense cloud with obstacles.

Three tests were carried out and are shown: 1) a simulation of a real field accident (the Macdona railroad accident in USA with the emission of huge amounts of chlorine); 2) a simulation of the Kit Fox experiments and 3) a comparison between the MicroSpray simulations and those of the CFD Mercure for the dispersion in presence of obstacles.

## 2. BRIEF OUTLINE OF THE MODELS

MicroSpray is part of the model system MSS that comprises MicroSwift (giving the 3D input wind field) and MicroSpray. MicroSwift is an analytically modified mass consistent interpolator over complex terrain. Given topography, meteorological data and buildings, a mass consistent 3D wind field is generated (Tinarelli et al., 2007). MicroSwift (Moussafir et al., 2004) is also able to derive a diagnostic turbulence (namely the Turbulent Kinetic Energy (TKE) and its dissipation rate) to be considered by MicroSpray inside the flow zones modified by obstacles. MicroSpray is a Lagrangian Particle Dispersion model derived from SPRAY (Tinarelli et al., 1994, 2000), able to account for the presence of obstacles or buildings, that are accounted for by setting as impermeable some of the cells of the terrain following grid where meteorological fields are defined. Dispersion is simulated following the motion of a large number of fictitious particles, whose velocity is split into two components: a mean one, or "transport-component", which is defined by the local wind reconstructed by MicroSwift, and a stochastic one, simulating the dispersion and reproducing the atmospheric turbulence, obtained by solving a 3-D form of the Langevin equation for the random velocity. The new MicroSpray version is especially oriented to deal with dense gas dispersion in urban environment and industrial sites. The new algorithms implemented into MicroSpray (Anfossi et al., in press; Tinarelli et al., in press) to simulate dense gas dispersion regard the following cases: plume with initial momentum (horizontal, vertical or oblique in any direction), plume without initial momentum and plume spread at the ground due to gravity.

The Mercure model (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. Mercure code has undergone extensive validation (see: Riou, 1987; Duijm and Carissimo, 2001). 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. A conservation relation for thermodynamic energy (enthalpy or virtual potential temperature) is optionally solved. Solving the thermal energy equation implies that thermal buoyancy (or dense) effects are included in the solution. Turbulence closure is by means of supplementary equations for the conservation of turbulent kinetic energy and dissipation using the k-ε model. The conservation equations are discretized using a combination of finite difference and finite-volume methods solving separately each type of operator. As default, the inlet boundaries are Dirichlet for all parameters and the outlet boundaries are zero gradient for all parameters. Important aspects of the Mercure setup for this study include: i) ideal gas equation of state, ii) Boussinesq approximation is used, implying that density variations only affect the flow through buoyancy (or dense) terms, iii) gravity is the only retained volume force (Coriolis effects are ignored), iv) thermal forcing due to radiative flux divergence is negligible.

## 3. MACDONA RAILROAD ACCIDENT

We refer to a study that compared the simulations by six widely-used hazardous gas models of downwind chlorine gas concentrations following three recent railcar accidents (Hanna, 2007). Being accidents that occurred at remote locations, no meteorological and concentration observations are available, thus source emissions rates were estimated and in that study it was not possible to investigate which model was "best". Plots and Tables of the results from the six models were produced and it was concluded that these models agree in their estimate of the downwind dispersion within an order of magnitude. Out of the three accidents we choose the case of Macdona (TX).

It was the aim of our work to run a MSS simulation with the input information from Hanna (2007) to verify if our prescribed concentrations were in accordance with those of the six models. In particular we computed the following quantities: maximum model-simulated 10 min average chlorine concentration at the downwind distances (0.1, 0.2, 0.5, 1 and 2 km), plume widths and the plume heights to the model-simulated concentration of 2000, 400, and 20 ppm at the same distances.

**Modelling implementation**

A computation domain of 2,200 m x 1,400 m x 1,000 m was considered. MicroSwift had horizontal grid spacing of 10 m and a stretched grid in the vertical. MicroSpray shared the same horizontal grid resolution. 100 particles were released per second from the 1 m source. The emission lasted 136 s, whereas the dispersion simulation lasted 30 minutes. Concentration was computed at 60 fictitious samplers per arc, from which the above quantities were estimated.

**Results**

An example of results is shown in Figure 1. It can be seen that the present results lie all within the variability of the ensemble of six models (Figures referring to the concentration of 2000 and 400 ppm, not shown, give the same result). Plume width is slightly large than the minimum of the six models, whereas in general plume height and concentration versus distance are closer to the median.

Lacking direct observations it is not possible to rank the seven (six plus MSS) model results. However, the results shown in Figure 1 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 the power law $C_2/C_1=(x_2/x_1)^{-p}$ with $p = 1.54$, that is in the expected range: 1.5-2 (Britter et al, 2002).

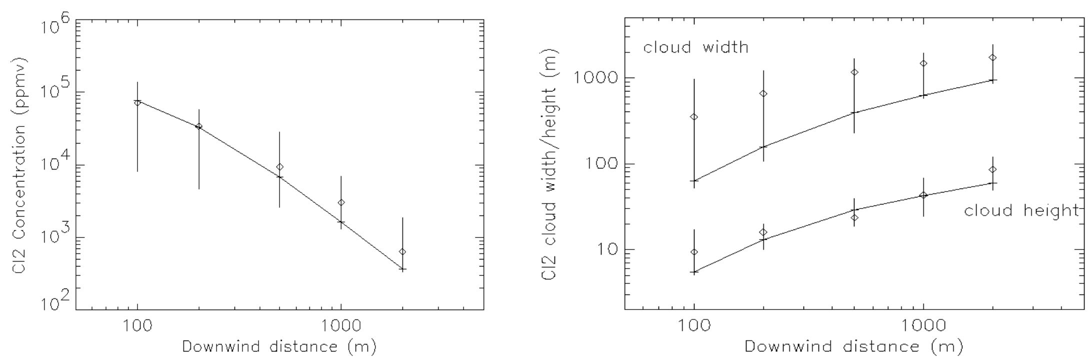


Figure 1. MSS results compared to the Macdona accident simulations from six widely-used models (from Hanna, 2007). Continuous lines indicate present results, the vertical bars show the variability (max, min) of the six models and circles locate the median of these models. Left graph refers to the Cl2 concentration versus distance; right graph plots Cl2 cloud width and height, both to the model-simulated concentration of 20 ppm versus distance.

## 4. KIT FOX EXPERIMENTS

Data and information on Kit Fox dense gas experiment were mainly found in MDA Database. The 1995 Kit Fox dense gas field data set consists of 52 trials where $CO_2$ gas releases were made thanks to a 1.5 m x 1.5 m ground level source over a rough surface during neutral to stable conditions. The relative emission density, $\rho_e/\rho_a$, where $\rho_e$ and $\rho_a$ are the emission and ambient densities respectively, was equal to 1.52. Depending on the considered trial, dense gas durations of release were representing short-duration transient puffs (about 2/3) or continuous plumes (about 1/3). 84 fast-response concentration monitors were located on four downwind arrays (25, 50, 100 and 225 m). Wind speeds and directions at 2 m levels, friction velocities and Monin-Obukhov lengths were provided for each of the 52 trials. In order to study the effects of increased roughness, the experiments used two sets of artificial roughness arrays: Uniform Roughness Array (URA) with a roughness length of about 0.01-0.02 m and Equivalent Roughness Pattern (ERP) with a roughness length of about 0.12-0.24 m.

**Modelling implementation**

A computation domain of 400 m x 240 m x 100 m was considered. MicroSwift had horizontal grid spacing of 2 m and a stretched grid in the vertical. MicroSpray shared the same horizontal grid resolution, while vertical grid spacing was 0.5 m up to 2 m above the ground. 10,000 particles were released per second from the 1.5 m x 1.5 m area source, whatever the duration

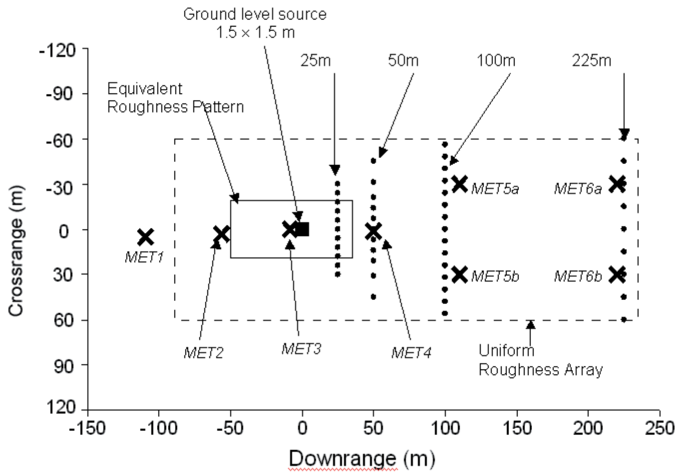


Figure 2. Plot plan of Kit Fox site (from Kit Fox MDA database).

of release. Concentration at sampler locations was computed. Roughness lengths of 0.015 m and 0.18 m were considered for the two sets of artificial arrays, that is to say respectively URA and ERP.

**Results**

Maximum predicted concentrations and observations have been compared, for a 20 seconds averaging times, at the different downwind distances. No limit of detection (LOD) has been used as lower bound for concentrations. Kit Fox trials can be split
into four groups, that is to say URA–continuous (12 trials), URA–puff (21 trials), ERP–continuous (6 trials) and ERP–puff (13 trials):

- URA–continuous: 2, 7 and 3 Pasquill - Gifford stability class D, E and F respectively
- URA–puff: 8, 5 and 8 Pasquill - Gifford stability class D, E and F respectively
- ERP–continuous: 1, 1 and 4 Pasquill - Gifford stability class D, E and F respectively
- ERP–puff: 6, 3 and 4 Pasquill - Gifford stability class D, E and F respectively

At the moment, only comparisons related to URA–puff and ERP–puff have been performed. Each of these two last groups has been statistically evaluated in order to determine the accuracy of MicroSpray model predictions with the observed data. Geometric mean bias (MG), geometric variance (VG), as well as factor of 2 (FA2) are presented in the following table.

Table 1. Statistical indexes related to maximum concentrations (20 seconds averaging time)

| Kit Fox experiment | URA - puff | ERP - puff |
|---|---|---|
| | 21 experiments | 13 experiments |
| MG | 1.11 | 1.11 |
| VG | 1.20 | 1.22 |
| FAC2 | 92.9% | 84.6% |

These results are quite encouraging and, in particular, well agree with those obtained by three different versions of the model HEGADAS (Hanna and Chang, 2001), and the CFD code FLACS (Hanna et al., 2004).

## 5. MICROSPRAY AND MERCURE SIMULATIONS OF DISPERSION IN PRESENCE OF OBSTACLES

These simulations were performed in two flow conditions: low wind speed (1.5 $ms^{-1}$ at 10 m) and higher wind speed (5 $ms^{-1}$ at 10 m). In both cases, a neutral turbulence was considered, thus assuming an input logarithmic wind profile. A regular obstacle (Lx=26.2 m, Ly=23.3 m and H=47 m) whose base center was located at 50 m downwind the emission stack (H=10 m, diameter = 4 m, vertical exit velocity of 1.14 $ms^{-1}$) was included in the domain (see Fig. 3). 10 $kgs^{-1}$ of a gas having relative emission density equal to 2.0 were emitted.

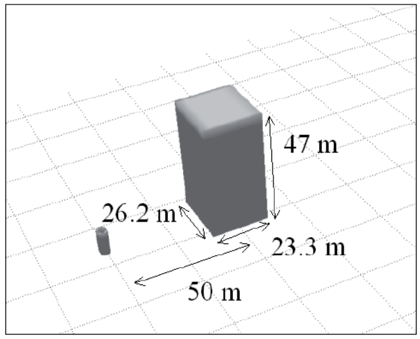


Figure 3. Plot of the dispersion situation simulated by Mercure and MicroSpray (MSS), in which the dimensions of the stack and obstacle are shown.

In Mercure simulations, a computation domain of 650 m x 550 m x 160 m was considered. The horizontal grid spacing is 0.7 m (near the release) up to 30 m. The vertical grid spacing is 2 m (near ground) up to 10 m. In Swift and MicroSpray the computation domain of 500 m x 200 m x 200 m was used and the horizontal grid spacing is 1 m whereas the vertical grid spacing is 0.5 m (near ground) up to 200 m above the ground.

Figure 4 shows ground level concentrations (g.l.c.) obtained in the two wind regimes by the two models. Concentrations are given in kg of pollutant per kg of air and pollutant mix. The overall shape of g.l.c. pattern is similar. However, we can notice two differences: i) MSS estimates more ‘counterflow’ motion near ground than Mercure and ii) at difference with Mercure, in the low wind speed case, MSS maximum is upwind the source. These differences might be due to the fact that the source (simulating a stack) is not explicitly considered as an obstacle by MSS while Mercure considered it both as a release and an obstacle. Another possible cause of these differences can be due to the gravity spreading algorithm used in MicroSpray. However, this algorithm seemed to work correctly in the above Macdona simulation and in the simulation of Thorney Island experiment 8 previously carried out (Anfossi et al., in press; Tinarelli et al., in press). Despite these differences, both models show a comparable splitting of the plume due to the presence of the obstacle, and, as expected, a large horizontal spread at ground due to the gravity effects, particularly evident in the lower wind speed case. At the base center of the obstacle, the width of the plume is, for low wind speed, 154 m with Mercure and 148 with MSS (considering 0.001 kg/kg iso-contour), and, for higher wind speed, 70 m with Mercure and 80 m with MSS (considering 0.002 kg/kg iso-contour). Also maximum ground level concentrations are comparable (they are particularly close to each other in the higher wind speed case) and the overall pattern of the impact at ground is very similar.

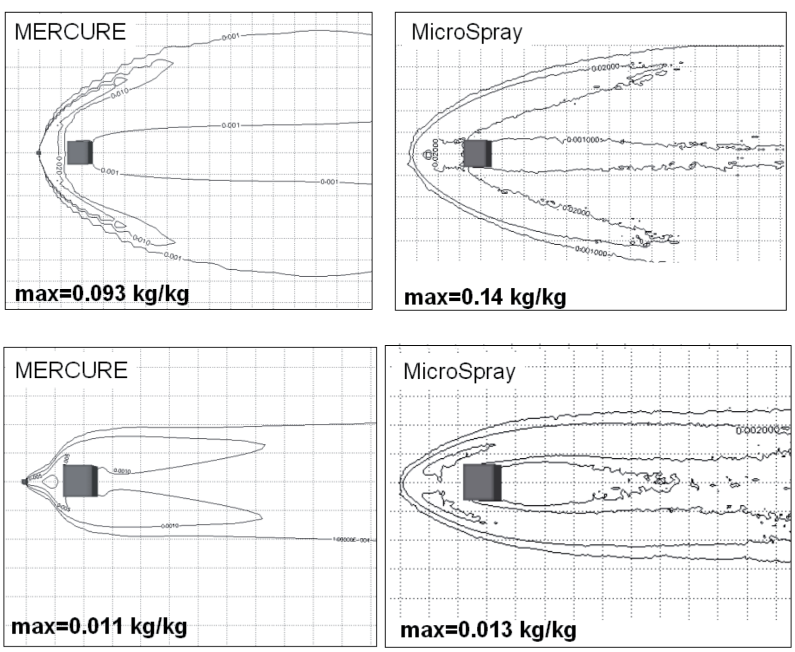


Figure 4. Glc obtained by Mercure and MicroSpray (MSS) in lower (above) and higher (below) wind speed.

## 6. CONCLUSIONS

In this paper we present the performances of the updated version of the Lagrangian particle dispersion model MicroSpray, that is especially dedicated to simulate the dense gas dispersion in presence of buildings, and other obstacles. MicroSpray performances are compared to a chlorine railway accident (Macdona), to a field experiment (Kit Fox) and to an atmospheric CFD model.

The previous results of this ensemble of comparisons, here presented, indicates that MicroSpray simulations are as accurate as simulations previously carried out with other models and thus can yield reliable estimates of dense gas dispersion.

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