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PROPOSAL FOR MODELLING THE DRY DEPOSITION OF SOLID PARTICLE AND GAS USING A 3D STOCHASTIC LAGRANGIAN DISPERSION MODEL

Ribstein Bruno[1], Cohen Elsa[1], Nibart Maxime[1] and Tinarelli Gianni[2]

[1] ARIA Technologies, 8, rue de la Ferme, F-92100 Boulogne-Billancourt, France
[2] ARIANET S.r.l., via Gilino 9, I-20128 Milano, Italy

Abstract: The deposit represents a flow of pollutants to the ground and depletes the plume. Dry deposition velocity models the soil's ability to retain the pollutant. ARIA/ARIANET in collaboration with CEA has developed the PSPRAY model, a Lagrangian 3D model of stochastic dispersion of pollutants in the atmosphere. A particle removal mechanism, linked to the stochastic equation solved by the model, is implemented to ensure that the dry deposition flux is proportional to the concentration at ground level. It is based on the calculation of a probability $P(h, \Delta t)$ that an amount of pollutants located at a certain height is absorbed during a certain time interval. The probability tends rapidly to zero when moving away from the ground level.

In this work we revise the implementation of this mechanism in the PSPRAY dispersion model. At each emission time step, the model emits virtual particles each carrying part of the emitted mass of pollutants. These virtual particles represent a set of solid particles or a certain volume of gas. In the presented work, an amount equal to $P(h, \Delta t) \cdot m_{par}$ is removed from the mass m_{par} carried by the particle. The proposed mechanism allows an identical treatment of the gas and solid particle cases. Thus, as the diameter of the solid particles tends towards zero, the deposition field approaches the one of a gaseous species.

Key words: *solid particles, dry deposition, lagrangian, modelling, PSPRAY, buildings***.**

INTRODUCTION

In the urban environment, exposure to air pollution is a major environmental problem. Pollutants are emitted from various sources and then dispersed (advection and diffusion) over a wide range of horizontal length scales. Microscale dispersion refers to processes acting on horizontal length scales smaller than about 5 km. Public health risk assessment requires modeling of pollutant dispersion in the atmosphere. This is not always sufficient, and it is sometimes necessary to model the deposition of pollutants on the ground, or on the facades of buildings. The deposition represents a flow of pollutants to the ground that depletes the plume. The dry deposition represents the capacity of the soil to retain pollutants, the wet deposition models the washout of the plume by raindrops.

ARIA/ARIANET in collaboration with CEA has developed the PSWIFT model in the Parallel-Micro-SWIFT-SPRAY (PMSS) system. The PSWIFT model is a mass-conserving diagnostic atmospheric model. PSPRAY is a (stochastic) 3D Lagrangian Particle Dispersion Model able to account for the presence of obstacles. They have been developed with the aim to provide a simplified, but rigorous solution of the flow and dispersion in industrial or urban environments in a short amount of time (Tinarelli et al., 1994, 2012).

The dry deposition model in Pspray was historically developed in 2 parts: for solid particles and then for (dense) gases. The 2 mechanisms are different, and the results obtained are possibly also different. We review the two mechanisms and present a unified mechanism for dry deposition for any type of pollutant. After this introduction, the dispersion modeling is presented, followed by the existing and proposed mechanism of dry deposition in Pspray. The numerical experiments are described and the results are analyzed. Finally, a summary reminds the important results obtained in this work.

DISPERSION MODELLING

There are three main families of deterministic atmospheric dispersion models: the Eulerian model, the Gaussian model and the Lagrangian model. An in-depth description of the models can be found in (Hanna et al., 1982) and Rodean (1996).

- Gaussian models are used to simulate the atmospheric dispersion of non-reactive pollutants near the source. They assume a Gaussian distribution around the center of the plume. The wind and the temperature are assumed to be stationary and uniform. Mass conservation is imposed in the plane transverse to the plume axis.
- Both Eulerian and Lagrangian models solve the advection-diffusion equation. The Eulerian viewpoint considers the evolution at a fixed point, i.e., at (x, y, z) constant. In each cell, the concentration evolution is given by the incoming and outgoing mass fluxes. The Lagrangian viewpoint follows a parcel of fluid in its displacement. The position is therefore not fixed, but the material volume always gathers the same set of fluid molecules over time.

In PSPRAY, the dispersion of an airborne contaminant is simulated by following the trajectories of a large number of numerical particles, each carrying a part of the emitted mass of pollutant. The trajectories are obtained by integrating in time the velocity of each numerical particle. The velocity of each particle is the sum of a component for the transport (average wind speed from PSWIFT), another one for the turbulence (stochastic contribution via the resolution of a Langevin equation) and of eventual parameterization taken into account (for example the gravitational settling).

Each numerical particle represents a set of molecules. For a pollutant flux Q in kg/h and N_{par} numerical particles emitted every dt_{min}, each particle will carry $m_{par} = Q \cdot dt_{min}/N_{par}$. Increasing the number of numerical particles improves the accuracy of the results, since each particle carries a smaller mass. The computation time depends linearly on the number of numerical particles and the average wind. Increasing the number of numerical particles therefore also results in an increase in computation time.

DRY DEPOSITION MODELING IN PSPRAY

The deposit represents a flow of pollutants to the ground and depletes the plume. In addition to the gravitational settling, the dry deposition velocity models the soil's ability to retain the pollutant. Dry deposition is modeled in a Lagrangian manner in PSPRAY, by computing the deposition probability of each numerical particle near the ground. Monin (1959) found a solution of the 1d advection-diffusion equation with the addition of a boundary condition reflecting the interaction with the surface and considering the gravitational settling. The solution $c_{unit}(z, t; h)$ is for an instantaneous point source of unit intensity at the height h. Let a parcel of pollutant initially at $z = h$ in $t = 0$. The probability $P(h, \Delta t)$ that this parcel is absorbed during the period Δt equals exactly the fraction of pollutant no longer in the air.

$$P(h, \Delta t) = 1 - \int_0^\infty c_{unit}(z, \Delta t; h) dz$$

Deposition in PSPRAY today handles a gas differently from a solid particle.
- For a gas, a mass equal to $m_{dep} = P(h, \Delta t) \cdot m_{par}$ is removed from the mass carried by the numerical particle and is deposited on the ground. The mass carried by the numerical particle is then $(1 - P(h, \Delta t)) \cdot m_{par}$.
- For solid particles, a random number Y is extracted from a uniform distribution. If the number is $Y < P(h, \Delta t)$ then the numerical particle is entirely retained by the soil. The deposited mass equals $m_{dep} = m_{par}$ and the numerical particle is no longer transported. If the number is $Y > P(h, \Delta t)$ the numerical particle acts as if no deposition is taking place, eventually reflecting off the ground. This is the mechanism initially presented in Boughton et al. (1987).

At periodic intervals, the mass in each mesh defining the computational domain is calculated. The concentration fields in $mass/m^3$ and deposition in $mass/m^2$ are thus estimated.

LIMIT AND MODIFICATION OF THE PSPRAY DEPOSITION MODEL

We have just explained the dispersion and deposition in the PSPRAY model. We now detail the limitations to the current deposition model. For solid particles, each numerical particle carries a mass $m_{par} = Q \cdot dt_{min}/N_{par}$. With numerical resolution $dx = dy = ds$, the deposited mass will never be less than that of a numerical particle, i.e. m_{par}/ds^2. Obviously, the higher N_{par} is, the lower this deposition threshold is. Gases do not have this threshold since the mass carried by a numerical particle is depleted by deposition.

Gravitational settling is taken into account for solid particles. Gravitational settling follows a Stockes law with a Cunningham correction factor. This velocity is proportional to d^2 with d the diameter of a solid particle. The velocity is of the order of $10^{-4}\, m/s$ for $d = 1\mu m$. Because the contribution of gravitational settling is negligible for solid particles of diameter $1\mu m$, the deposition should be equivalent to that of a gas emitted in the same quantities. Figure 1 illustrates the threshold effect and shows that this is currently not the case in PSPRAY. There are 2 pollutants considered, a gas and fine particles of diameter $1\mu m$.

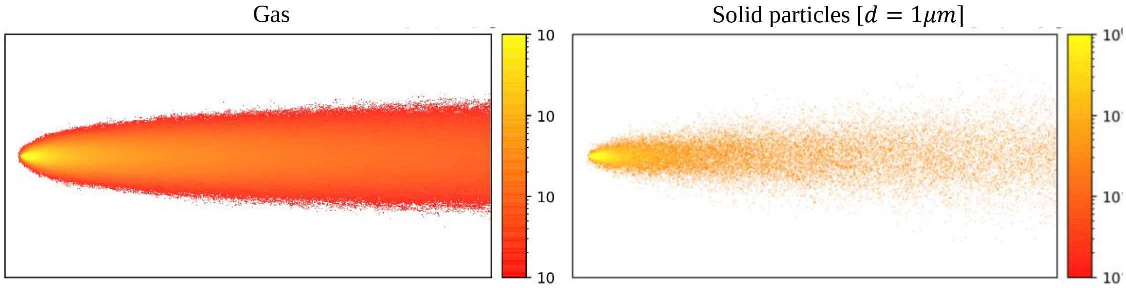

Figure 1: Dry deposition for a gas and solid particles with d=1µm (old mechanism)

Figure 2 shows the deposition along the plume axis by changing the number of digital particles emitted. It illustrates the threshold effect as the threshold decreases by increasing N_{par}. In the case $N_{par} = 100$, the computation time is 19s on 10 processors, but it increases to 160s with $N_{par} = 1000$.

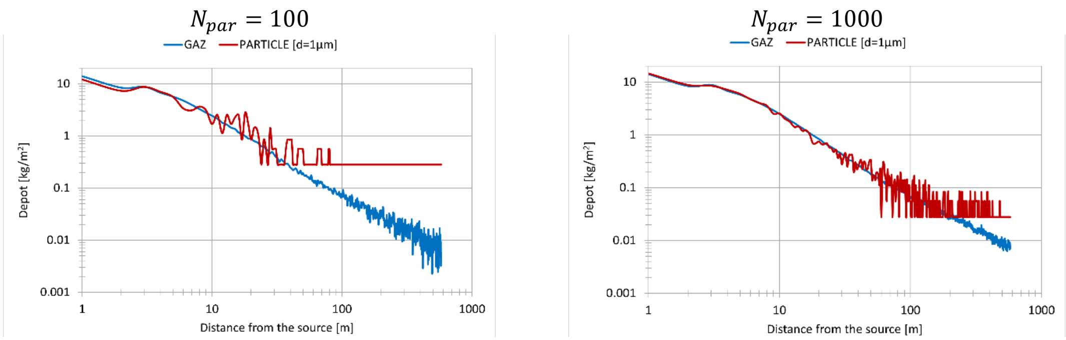

Figure 2: Dry deposition along the plume for a gas and solid particles with d=1µm (old mechanism)

The deposition probability already takes into account the gravitationnal settling and the deposition velocity. The proposed deposition mechanism is to use the one currently in place for gas.

DESCRIPTION OF THE NUMERICAL EXPERIENCES

The proposed deposition mechanism is verified in an idealized setting, and where a comparison to a Gaussian model is possible. This is the method also used by Boughton et al. (1987), and we use the same Gaussian model, namely Ermak (1977).

- The modeled domain does not include any obstacle and it covers an area of $600m \times 300m$, at the resolution of $dx = dy = 1m$.
- The weather conditions are slightly unstable. The temperature gradient is $-1.8\,°C/m$ and the wind profile follows a $u(z) = u_0(z/z_2)^\alpha$ law, with $z_2 = 10m$, $u_0 = 4\,m/s$ and $\alpha = 0.15$.
- A source emits a continuous flow of pollutant $Q = 10^4 kg/h$ from a height $h = 1m$. The emitted species are a gas and solid particles of diameter $1\mu m$, both have a deposition velocity $v_d = 0.1\,m/s$. $N_{par} = 1000$ numerical particles are emitted every $dt_{min} = 10s$.

Wind is uniform in the Gaussian model used, which is not the case in PSPRAY. For the Gaussian model, we choose $\sigma_z(x) = \sigma_y(x) = 0.36(x)^{0.86}$, equivalent to a B1 case of the Brookhaven National Laboratory classification. The wind chosen is $u_0 = 4\,m/s$.

RESULTS

Figure 3 shows the concentration along the plume. The concentrations in PSPRAY are estimated in a layer $dz = 2m$. With the Gaussian model, the concentration is calculated at $z = 1m$. The concentration for gas and small particles are similar, and they remain within a factor of 2 of the Gaussian model from a distance of $20m$ from the source. The concentration is obtained by PSPRAY by counting N_{snap} times the mass contained in each cell. The smallest modeled concentration equals m_{par}/N_{snap}, i.e. when a numerical particle is counted only once. This corresponds to the fluctuations shown in Figure 3.

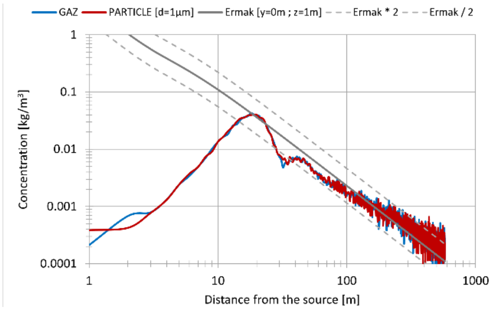

Figure 3: Concentration along the plume for PSPRAY and the Ermak (1977) Gaussian model

Figure 4 shows the deposition field along the plume, and also along the transverse axis for 2 distances from the source: $x = 100m$ and : $x = 200m$. With the proposed deposition mechanism, the deposition fields for gas and solid particles of diameter $1\mu m$ are now similar. The deposition along the plume remain within a factor of 2 from a distance of $10m$ from the source. The deposition given by the Gaussian model is increasingly smaller compared to that modeled PSPRAY. The transverse spread of the plume in the Gaussian model is increasingly larger compared to that in PSPRAY. These two observations suggest that the PSPRAY model appears to be slightly less dispersive than the Gaussian model. The weather conditions and the turbulence estimation are different in the 2 models. The study was not an inter-comparison of the 2 models, and we did not investigate this further.

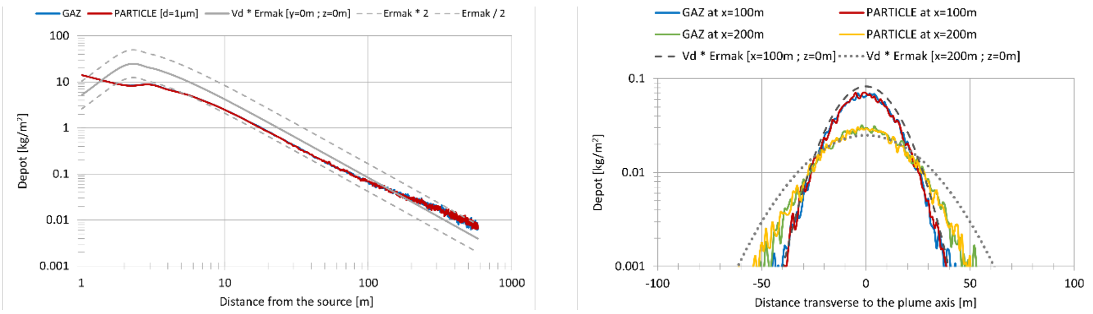

Figure 4: Dry deposition along the plume and along the transverse axis for a gas and solid particles with d=1µm for PSPRAY (new mechanism) and the Ermak (1977) Gaussian model

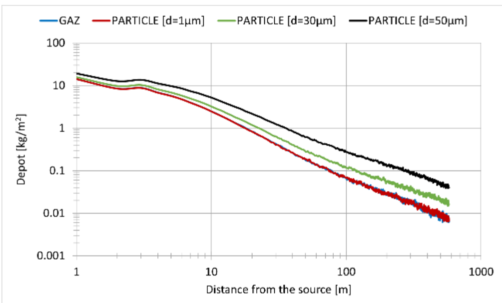

Figure 5: Dry deposition along the plume for a gas and solid particles with different diameters (new mechanism).

Finally, the figure 5 shows the evolution of the deposition for the gas and for solid particles of different diameters $d = 1\mu m$, $30\mu m$ et $50\mu m$. The gravitational settling evolves as d^2, and is approximately $10^{-4}\ m/s$ for $d = 1\mu m$. It remains negligible for $10\mu m$, but then begins to become significant.

ILLUSTRATION OF THE IMPACT OF A BUILDING

The PSPRAY model has been developed to take into account the presence of possible obstacles. With meteorological conditions similar to the previous case, the figure 6 illustrates that the presence of obstacles does not change the previous conclusions. The concentration and deposition fields for a gas and solid particles of diameter 1µm remain similar.

X-Z section of gas concentration and X-Y section of dry deposition

X-Z section of solid particles [$d = 1\mu m$] concentration and X-Y section of dry deposition

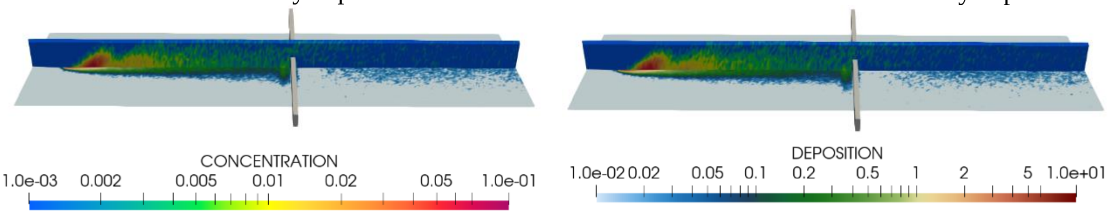

Figure 6: illustration of the impact of a building on concentration and deposition

CONCLUSION

The PSPRAY dry deposition mechanism was different for fine particles and gases. A unique dry deposition mechanism is proposed and tested on an academic configuration, and comparisons performed against a rectilinear Gaussian model. An illustration shows that the new deposition mechanism is compatible with obstacles.

In an urban environment, deposition on facades can also be significant. Although this can be modeled by the PSPRAY model, this depletion has not been analyzed. The deposition mechanism of the PSPRAY model is compared to that of a more idealized model. In order to validate the deposition model, it will be interesting to compare it to a measurement campaign, and to a more complex model than PSPRAY.

REFERENCES

Tinarelli G., Anfossi D., Brusasca G., Ferrero E., Giostra U., Morselli M.G., Moussafir J., Tampieri F., Trombetti F., 1994. Lagrangian particle simulation of tracer dispersion in the lee of a schematic two-dimensional hill. *J. Appl. Meteorol*. 33 (N. 6), 744–756.

Tinarelli G., Mortarini L., Trini Castelli S., Carlino G., Moussafir J., Olry C., Armand P., Anfossi D., 2012. Review and validation of Micro-Spray, a Lagrangian particle model of turbulent dispersion. In: Lin, J., Brunner, D., Gerbig, C., Stohl, A., Luhar, A., Webley, P. (Eds.), Lagrangian Modeling of the Atmosphere. vol 200. *Geophysical Monograph, American Geophysical Union*, Washington DC, pp. 311–327

Hanna, S.R., Briggs, G.A., Hosker, R.P., 1982. Handbook on Atmospheric Diffusion. DOE/TIC-11223. *Department of Energy*, pp. 102.

Rodean, H.C., 1996. Stochastic Lagrangian Models of Turbulent Diffusion, vol 45 American Meteorological Society, Boston, USA.

Monin, A. S., 1959: On the Boundary Condition on the Earth Surface for Diffusing Pollution, *Adv. Geophys*. 6,435-436.

Boughton B.A., Delaurentis J.M., Dunn W.E. [1987]. A Stochastic model of particle dispersion in the atmosphere. *Boundary-Layer Meteorology* 40, 147-163.

Ermak, D. L.,1977: An Analytical Model for Air Pollutant Transport and Deposition from a Point Source, *Atmospheric Environment*, 11, 231-237.