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**ADAPTATION OF THE LAGRANGIAN MODULE OF A CFD CODE FOR ATMOSPHERIC  
DISPERSION OF POLLUTANTS IN COMPLEX URBAN GEOMETRIES AND COMPARISON  
WITH EXISTING EULERIAN RESULTS**

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**Abstract:** In the general context of atmospheric dispersion in urban neighborhood or around an industrial site, Lagrangian models consist in calculating and tracking the trajectories of particles of pollutant emitted into the turbulent atmosphere. These models are particularly suitable for the study of complex, unsteady or inhomogeneous flows, which is precisely the case of atmospheric flows in urban areas and complex industrial sites. They are also recommended to deal with dispersion near the sources. Usually, these models use wind and turbulence fields computed by an external code. In this work, the objective is to compare the Lagrangian and the Eulerian atmospheric dispersion modules in the same Computational Fluid Dynamics (CFD) open source code (*Code\_Saturne*), therefore using the same wind and turbulence field for both. For each simulation we want to compare the turbulent dispersion of pollutants obtained with the Lagrangian approach to the existing results previously obtained with the Eulerian methods. The stochastic Lagrangian model used in this work is the *Simple Langevin Model* (SLM) of Pope (2001) and pertains to the approaches referred to as PDF (Probability Density Function) methods. To our knowledge, this formulation of model has not previously been used in the context of atmospheric dispersion. In this paper, we first show that our model respects the well-mixed criterion. Then, we validate our model in the case of a continuous punctual release with uniform mean wind speed and turbulent diffusivity, by checking with the existing analytical solution. Finally, we validate the model with several experimental campaigns, considering atmospheric stratification and buildings. The first field experiment program considered in this paper has been conducted on the ‘SIRTA’ site (*Site Instrumental de Recherche par Télédétection Atmosphérique*), in the southern suburb of Paris, and involves a stably stratified surface layer.

**Key words:** *atmospheric dispersion, Lagrangian stochastic modelling, turbulence, CFD*

## INTRODUCTION

A cloud of pollutants released into the atmosphere is subject to three main processes: advection, diffusion and surface deposition. By definition, the turbulent dispersion is characterized by the combination of advection and turbulent diffusion. This phenomenon is highly dependent on turbulent flow characteristics. There is indeed a wide range of eddies in the atmospheric boundary layer and they all participate in their own way to the transport and diffusion of the cloud. In particular, the turbulent dispersion of the pollutants is not as effective close to the emission source as opposed to further away: the difficulty of its modelling therefore amounts to correctly take into account the effect of the different turbulent structures. In this work, the focus is on the atmospheric dispersion modelling at local scale (urban or industrial sites), *i.e.* for distances of the order of a few kilometers.

The Eulerian models of dispersion are based on the resolution of the advection-diffusion equation on a scalar field corresponding to the concentration of pollutant. This is done by performing a discretization of this equation in time and space on a mesh. Eulerian models have been used so far at EDF R&D (*Electricité de France*) to model atmospheric dispersion, by means of the CFD code *Code\_Saturne* and making use of its atmospheric module. On the other hand, the Lagrangian models consist in calculating and tracking the trajectories of particles in a turbulent flow. The cloud of pollutants is discretized and described by a large number of particles emitted into the atmosphere. In this work, the objective is to make use of both the Lagrangian and the atmospheric module of *Code\_Saturne* to model the turbulent dispersion of pollutants with the Lagrangian approach and compare it to the existing results previously obtained with the Eulerian methods.

## METHODOLOGY

*Code\_Saturne* (<http://code-saturne.org/>) is an open-source CFD code, developed at EDF R&D since 1997. It solves the general equations of fluid mechanics (*i.e.* continuity equations, momentum, energy and turbulence)

using numerical methods and turbulence models. These equations are solved on all types of meshes, including complex unstructured meshes. More details on the numerical methods implemented in the code are provided in Archambeau et al. (2004).

The methodology for stationary dispersion simulations in *Code\_Saturne* is the following. We perform two calculations. The first calculation is used to calculate the dynamical mean fields associated to the wind flow ("continuous phase"): velocity, pressure, temperature and turbulence. Once the steady state is reached, this calculation is stopped. The second calculation simulates the dispersion of pollutants within the pre-calculated flow field ("dispersed phase"), thus at frozen velocity, pressure and temperature and turbulence fields. The Eulerian and Lagrangian methods used in our work for the dispersion calculation are detailed subsequently. The turbulence models used for our studies are RANS models with classical  $k-\varepsilon$  or  $R_{ij}-\varepsilon$  closures adapted to the atmosphere and complex geometries.

### Eulerian approach

If we consider a species of concentration  $c$  within the pre-calculated flow (assumed to be incompressible), *Code\_Saturne* will solve the following advection-diffusion equation:

$$\frac{\partial \bar{c}}{\partial t} + \bar{U}_{f,j} \frac{\partial \bar{c}}{\partial x_j} = \frac{\partial}{\partial x_j} \left( D \frac{\partial \bar{c}}{\partial x_j} - \overline{U'_{f,j} c'} \right) + \bar{S} + \bar{R} \quad (1)$$

where  $\bar{U}_{f,j}$  is the mean velocity of the fluid along the  $j$  axis,  $D$  the molecular diffusivity,  $\bar{S}$  and  $\bar{R}$  respectively the source and reactive terms.

### Lagrangian approach

Let  $\vec{X}_p(t)$  be the position of a particle included in the carrier flow at a time  $t$ . Then:  $d\vec{X}_p = \vec{U}_p(t)dt$ .

The movement of each particle included in the carrier flow described by  $\vec{U}_p(t)$  is governed by Newton's second law. Assuming heavy particles, with a diameter of the same order of magnitude as the Kolmogorov length scale, the equation obtained on the particle velocity is (Minier and Peirano, 2001):

$$\frac{d\vec{U}_p}{dt} = \frac{\vec{U}_s - \vec{U}_p}{\tau_p} + \vec{g} \quad (2)$$

where  $\vec{U}_s$  is the velocity of the fluid sampled through the trajectory of the particle ( $\vec{U}_s(t) = \vec{U}_f(\vec{X}(t), t)$ ), and  $\tau_p$  the relaxation timescale of the particle. When  $\tau_p$  tends to zero,  $\vec{U}_s$  tends to  $\vec{U}_p$  and we reach in the limit case of fluid particles. Thus, every type of particles can be simulated, from gaseous particles to particulate matter.

As we calculate the wind flow with RANS models, we only have access to the statistical mean value of  $\vec{U}_s$ . Thus, in order to close (2), we need to reconstruct the turbulence effects: this is done by introducing a stochastic differential equation modelling the evolution of  $\vec{U}_s$ .

### The Simple Langevin Model (Pope, 2001)

For the sake of simplicity, let us consider the case of fluid particles, *i.e.*:  $\vec{U}_s = \vec{U}_p$ . Then the simple Langevin model writes as follow:

$$dU_{p,i} = -\frac{1}{\rho} \frac{\partial \bar{P}}{\partial x_i} dt - \frac{U_{p,i} - \bar{U}_{f,i}}{T_L} dt + \sqrt{C_0 \bar{\varepsilon}} dW_i \quad (3)$$

where  $\frac{\partial \bar{P}}{\partial x_i}$  is the mean pressure gradient,  $C_0$  a constant,  $\bar{\varepsilon}$  the mean dissipation and  $dW_i$  a Wiener process

of mean 0 and variance  $dt$ . Also:  $T_L = \frac{1}{\frac{1}{2} + \frac{3}{4} C_0} \frac{k}{\varepsilon}$  is the "Lagrangian timescale" which actually stands for a

particle return-to-equilibrium timescale. In the case of the simple Langevin model, it is isotropic.

To our knowledge, this formulation of model with the pressure gradient has not previously been used in the context of atmospheric dispersion. There are several reasons why we have chosen to go further developing it. First, it is written in terms of instantaneous velocity which allows a very simple formulation with the mean pressure-gradient term clearly included in the drift term. It should be highlighted that the presence of this mean-

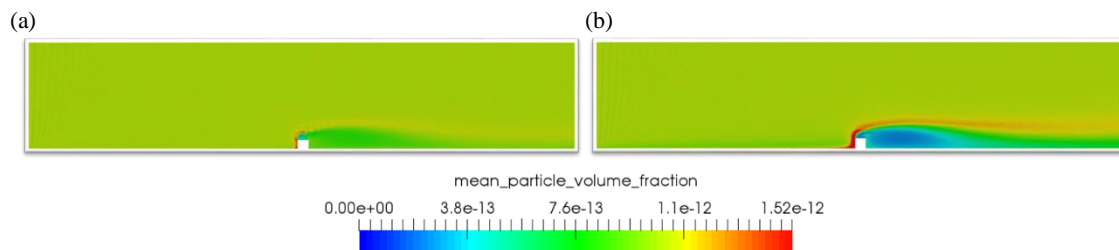
pressure gradient term is what allows the mean-continuity equation to be respected and thus ensures the model to be free of spurious drifts (Minier et al., 2014). In comparison, to make up for observed spurious drifts in their models, written in terms of fluctuating velocity, several authors heuristically added *ad-hoc* drift terms. This made the formulation of their models much more complex than if they were written in terms of instantaneous velocity only with the pressure-gradient term. Indeed, the latter formulation requires the calculation of only 3 gradients, one for each direction, instead of 27 with the formulation written in terms of fluctuating velocity, used by Thomson (1987) for example. Moreover, by construction (see Pope, 2001), the simple Langevin model ensures full consistency with the mean Navier-Stokes and the Reynolds equations with Rotta's closure. Finally, no hypothesis is made on the PDF of the velocity of the particles, which was not the case of many of the former models used in the atmospheric literature. For instance, Thomson (1987)'s model assumed the PDF to be Gaussian, but this hypothesis is no longer valid when we move to convective atmospheric boundary layer cases. In our case, the PDF is a result of the model.

### WELL-MIXED CRITERION

The well-mixed criterion states that an initially uniform particle concentration in a turbulent flow should remain uniform. In this section, we will show that our model respects this criterion. We studied two cases respectively corresponding to homogeneous and inhomogeneous turbulence. For the case with homogeneous turbulence we found that the criterion was well satisfied (not shown). We present here the case of inhomogeneous turbulence which involves an obstacle within a boundary layer (see figure 1). Given the stationary flow corresponding to this situation, we first initialized the domain with uniform particle concentration. Then, we injected, at the inlet, a uniform particle concentration field. We then observed the temporal evolution of the particles (subjected to the mean velocity and turbulence fields relative to the carrier fluid). After a transient time where the particles mix in the domain, a stationary state is reached (the number of particles in the simulation no longer varies). The objective is to see if the concentration remains uniform over time.

One point is to be made here, answering the following question: what happens if the pressure-gradient term is not properly taken into account in the Langevin equation? (Indeed, it has not always been the case in previous atmospheric Lagrangian models, see previous paragraph.)

To answer this question, two configurations are examined. Configuration (a) corresponds to the simulation with a properly taken into account pressure-gradient term and the use of the fully consistent  $R_{ij}-\epsilon$  Rotta model. Configuration (b) is the same as configuration (a), only removing the pressure-gradient term from the Langevin equation. The configuration (a) shows a uniform (the error compared to the ideal uniform case is not shown here but is about 4% and is mainly due to small discrepancies around the obstacle). Obviously the removal of the pressure-gradient term (configuration 2) leads to important spurious drifts upstream and downstream the obstacle (error: 16%). This simulation highlights the fact that the pressure-gradient term, as it is such that the mean velocity field satisfies the divergence-free condition, is what makes it possible to maintain a uniform concentration.



**Figure 1.** Mean concentration field. From left to right: (a) Taking into account pressure-gradient term and the fully consistent  $R_{ij}-\epsilon$  Rotta model. – (b) No pressure-gradient term and the fully consistent  $R_{ij}-\epsilon$  Rotta model.

### VALIDATION CASE: CONTINUOUS POINT RELEASE WITH UNIFORM MEAN SPEED AND TURBULENT DIFFUSIVITY

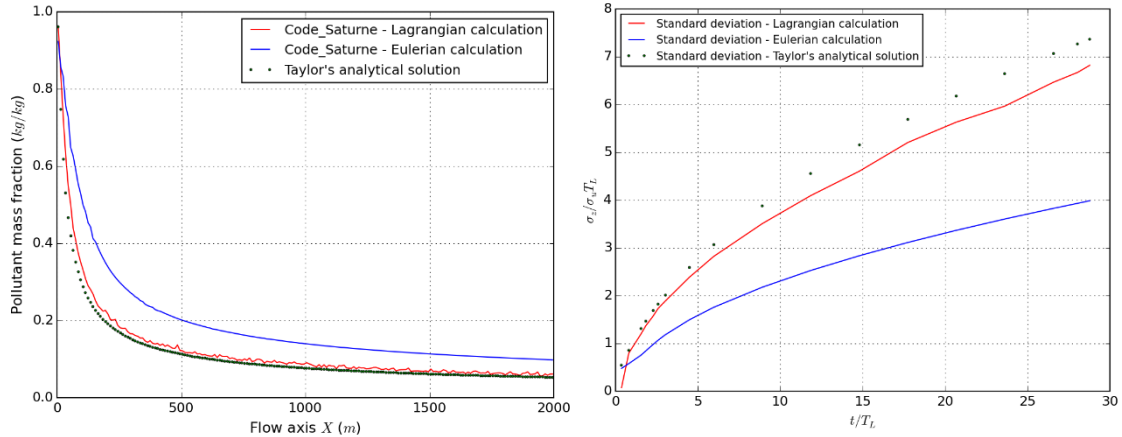
In this section, the objective is to validate our model in the case of a continuous point release (mass flow rate:  $Q$ ), under uniform mean wind speed and homogeneous turbulence conditions. This study is of interest because under these conditions, there is an analytical solution. It is therefore an opportunity for us to compare our Lagrangian model with this solution, as well as to observe the differences with the Eulerian model. The solution was first obtained by Taylor (see Arya, 1996) with some hypothesis on the form of the autocorrelation function, for the field of maximum concentration as a function of the distance to the source  $x$  is the following:

$$\bar{c}_{\max}(x) = \frac{Q}{\sqrt{2\pi}\bar{U}_{f,x}\sigma_z(x)} \quad (4)$$

where  $\sigma_z(x)$  is the plume standard deviation, formulated as follow:

$$\sigma_z(x) = \sigma_{U_{f,x}}(x) \frac{x}{\bar{U}_{f,x} \sqrt{1 + \frac{x}{2\bar{U}_{f,x}T_L}}} \quad (5)$$

This formulation, used in numerous atmospheric dispersion codes, allows the well-known discrimination of near-field/far-field regimes of diffusion (see Arya, 1996). Figure 2 shows the maximum concentration along the flow axis and compare both the Eulerian and Lagrangian approaches to the analytical solution previously introduced.

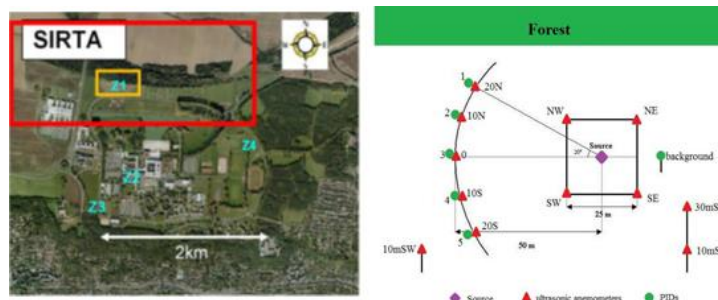


**Figure 2.** Mean concentration field. From left to right: (a) Maximum concentration along the flow axis. – (b) Adimensionalized plume standard deviation along the flow axis.

The Lagrangian model provides here much more accurate results than the Eulerian model. This is due to the fact that this Eulerian model (RANS 1<sup>st</sup> order) does not take into account the different diffusion behaviors between near and far fields. In the near field, there is a rapid spread, while far from the source, the diffusion is slower. This is of course taken into account in the analytical solution through the formulation of the standard deviation (see equation (5)). By construction – demonstration not shown here, see Pope (2001) for details –, this characteristic is also intrinsically included in our Lagrangian model. Figure 2 shows that near the source, there is a sharp and significant drop in concentration for the Lagrangian model and the analytical solution, which means rapid diffusion, whereas the Eulerian model diffuses much more slowly. On the other hand, far from the source, there is a quasi-parallelism between our three curves, which reflects an identical diffusion whatever the approach: we retrieve the theoretically well-known proportionality of the plume concentration standard deviation to the distance from the source. One important point to be remembered here is that the Eulerian model used for the calculation of turbulent scalar fluxes is an SGDH (Simple Gradient Diffusion Hypothesis) model, which uses a first-order closure for the dispersion equation. A DFM (Differential Flux Model), that is a full second order RANS model, should yield results more similar to the analytical solution, since it is a second-order closure that completely transports the turbulent scalar fluxes. However, this model is not completely developed and has not yet been used in atmospheric dispersion studies.

### INDUSTRIAL CASE: SIRTÀ

The SIRTÀ (*Site Instrumental de Télédétection Atmosphérique*) site, located in the southern suburb of Paris, is a complex site containing buildings, a lake and more or less dense vegetation. In our work, the objective is to simulate in *Code\_Saturne* a near-field (50 to 200 m) dispersion experiment carried out on this site by Wei et al. (2016). The experimental campaign involved a stably stratified surface layer and an almost easterly wind. Figure 3 shows a view from the top of the SIRTÀ site, with a representation of its different zones. The campaign we study is located in zone 1 (in yellow on the figure) and the simulation domain is shown in red on the figure. This area is bounded by a forest to the north and a road to the south. The mesh for the modelling area and the position of the source and the device instruments are also shown in figure 3.



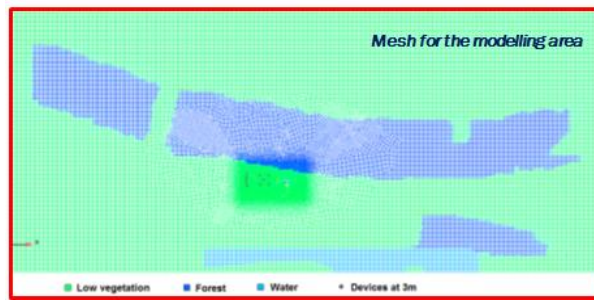


Figure 3. Sirta site's map, instrumental devices and mesh (horizontal cross section) for the modelling area.

The results here are still under investigations and will not be developed. Figure 4 shows these preliminary results through the comparison of the mean concentrations ( $ppmv$ ) between measurements and simulations for the five points of measurements described in figure 3 (green points corresponding to the 'PID' caption).

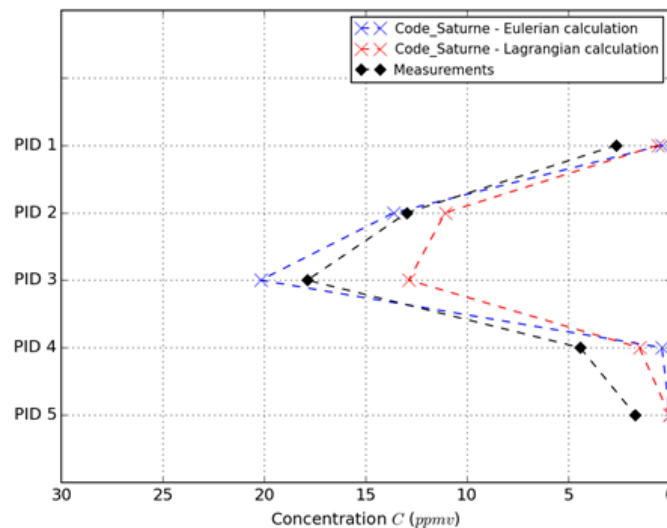


Figure 4. Comparison of the mean concentrations ( $ppmv$ ) between measurements and simulations.

## CONCLUSION

The objective of this work is to develop a Lagrangian stochastic tool to simulate atmospheric dispersion simultaneously with Eulerian dispersion, within the CFD code *Code\_Saturne*. After choosing to work with the *Simple Langevin Model* of Pope (2001), we validated our model for several situations. First we ensured that our model respects the well-mixed criterion, considering the case of both homogeneous and inhomogeneous turbulence. Then we validated the model by checking with an analytical solution and showed indeed the well-known distinction by the model of the two regimes of diffusion (near and far fields). Finally, to this date, we are currently validating the model for several industrial cases. Preliminary results were shown in this paper for the Sirta campaign. We are also currently working on validating the model on the MUST campaign (*Mock Urban Setting Test*), which was conducted on Utah's desert, USA, and involves obstacles.

## REFERENCES

- Archambeau, F., Méchitoua, N. and Sakiz, M., 2004: Code Saturne: A finite volume code for the computation of turbulent incompressible flows-Industrial applications. *International Journal on Finite Volumes*.
- Arya, S. P., 1999: *Air pollution meteorology and dispersion* (Vol. 6). Edition, New York: Oxford University Press.
- Minier, J. P., Chibbaro, S. and Pope, S. B., 2014: Guidelines for the formulation of Lagrangian stochastic models for particle simulations of single-phase and dispersed two-phase turbulent flows. *Physics of Fluids*.
- Minier, J. P. and Peirano, E., 2001). The PDF approach to turbulent polydispersed two-phase flows. *Physics Reports*, **352**(1), 1-214.
- Pope, S. B., 2001: *Turbulent flows*. Edition, Cambridge University Press.
- Thomson, D. J., 1987: Criteria for the selection of stochastic models of particle trajectories in turbulent flows. *Journal of Fluid Mechanics*, **180**, 529-556.
- Wei, X., Dupont, E., Carissimo, B., Gilbert, E. and Musson-Genon, L., 2016 : Near-Field Pollutants Dispersion in a Stratified Surface Layer: Comparison of Numerical Study and Field Measurements of Sirta. *Air Pollution Modeling and its Application XXIV*, 365-369.