22nd International Conference on
Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes
10-14 June 2024, Pärnu, Estonia

A NEW OPERATIONAL MICROMIXING APPROACH TO MODEL CONCENTRATION FLUCTUATIONS

Lionel Soulhac[1], Guillevic Lamaison[2], Perrine Charvolin[2], Chi Vuong Nguyen[2], and Patrick Armand[3]

[1] INSA Lyon, CNRS, Ecole Centrale de Lyon, Universite Claude Bernard Lyon 1, LMFA, UMR5509, 69621, Villeurbanne, France
[2] Ecole Centrale de Lyon, CNRS, Universite Claude Bernard Lyon 1, INSA Lyon, LMFA, UMR5509, 69130, Ecully, France
[3] CEA, DAM, DIF, F-91297 Arpajon, France

Abstract: In the framework of the Building Urban & Industrial Lagrangian Dispersion (BUILD) model, a new micromixing model for the concentration fluctuations is proposed. We assume a clipped probability density function for the concentration, considering that the Lagrangian particles coming from the source sample the upper part of the concentration distribution. The lower part of the distribution is supplemented to ensure the average concentration. We show that this approach is theoretically more rigorous than the volumetric approach of Cassiani (2013) and we validate that it satisfactorily represents the moments of the fluctuations, in the case of a Gamma type distribution. This new micromixing model is then implemented in the BUILD model. We discuss comparisons with the experimental data of Marro et al. (2018) and evaluate the ability of the approach for application in fast response modelling for crisis management.

Key words: *Concentration fluctuations, Lagrangian dispersion modelling, emergency response*

INTRODUCTION

Modelling concentration fluctuations in a pollutant plume is an important problem for the prediction of doses associated with non-linear toxicological effects, for exceedances of explosivity or flammability thresholds or for odours evaluation. Different approaches have been developed in the literature to model or simulate concentration fluctuations (Cassiani et al., 2020): Eulerian DNS, LES or RANS models, PDF methods (micromixing models), Lagrangian Two-Marked-Particles Methods, heuristic models or analytical and phenomenological approaches. They allow, depending on their complexity, to describe instantaneous fluctuations or to characterize the statistical distribution of these fluctuations, in real complex flows or in much simpler academic configurations. A significant limitation of most of these approaches is their computational cost, which makes it difficult to use in an operational context on complex urban or industrial configurations.

Cassiani (2013) proposed an original heuristic approach to model the variance of concentration, using a Lagrangian macromixing model coupled with a so-called “volumetric” micromixing approach, making it possible to calculate the variance of concentration fluctuations with a limited additional computational cost. Despite relatively satisfactory results in comparison to measurements (Marro et al., 2018), Cassiani's approach presents significant conceptual issues and does not allow to properly describe the higher order moments of the fluctuation distribution. In the present work, we propose a new model to correct some limitations of this approach.

MODEL DESCRIPTION

In a turbulent flow, the concentration fluctuates in space and time under the effect of the spectrum of turbulent scales. Using Reynolds decomposition, the instantaneous concentration c can be decomposed into the sum of the average concentration $\bar{c}$ and the concentration fluctuation c':

$$c = \bar{c} + c' \tag{1}$$

The simulation of the average concentration $\bar{c}$ by a stochastic Lagrangian particles model is called "macro-mixing modelling" because the evolution of the average concentration is driven by the large scales of turbulence. The detailed simulation of the instantaneous fluctuation is much more complex because it evolves under the effect of micro-scales which can only be simulated by resolving the very small eddies of the flow, leading to a prohibitive computational cost (DNS - Direct Numerical Simulation approach). Therefore, different approaches have been developed to model concentration fluctuations (Cassiani et al., 2020), which aim not to reproduce instantaneous variability but only the statistical distribution of fluctuations, through its Probability Density Function (PDF) and its main moments. As an example, the Probability Density Function associated with different concentration signals is shown on **Figure 1**.

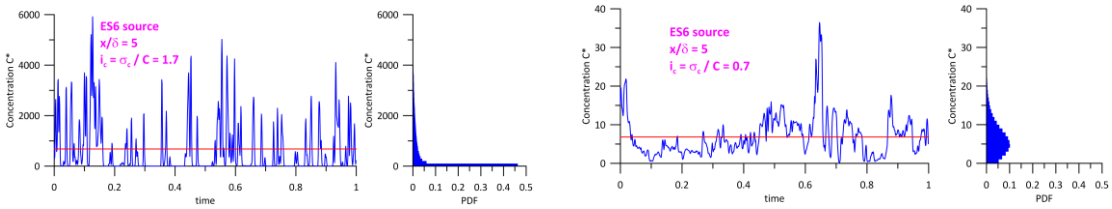


Figure 1. Time evolution and probability density function (pdf) of the concentration fluctuations (from Marro et al., 2018). Near field (left) and far field (right).

Micro-mixing model

Among the existing approaches, the micro-mixing model is compatible with Lagrangian particle dispersion models. It aims to solve a transport equation for the concentration PDF explicitly taking into account the dissipative effects of molecular diffusivity. The micro-mixing model is based on the introduction of a Lagrangian variable C representing the concentration associated with each particle, the evolution of which is given by a generic relation of the form:

$$\frac{dC}{dt} = \phi(C, X, U', t) \tag{2}$$

where the ϕ function takes into account the attenuation of the concentration variance. The IECM model for ϕ (Interaction by Exchange with the Conditional Mean, Pope, 1998) assumes the following parameterization:

$$\frac{dC}{dt} = -\frac{C - \overline{(C|X,U)}}{\tau_m} \tag{3}$$

where $\overline{(C|X,U)}$ is the mean concentration conditioned on the local position and velocity and τ_m represents the time scale of local mixing, which is defined as a function of the local velocity variance, the average dissipation rate of turbulent kinetic energy, the size of the source and the flight time of the particles (Cassiani et al., 2005). This model has the desirable property of leaving the average concentration field unchanged and it has been used to simulate the PDF of concentration fluctuations in the case of atmospheric dispersion from localized sources (Postma et al., 2011).

Volumetric micro-mixing model

Due to the need to simulate particle trajectories for all the flow, the classical micro-mixing model is very computationally expensive and it is not suitable for a fast-response operational tool. Therefore, Cassiani (2013) proposed an approach, called "volumetric micro-mixing model", which significantly reduces the computational cost, by simulating only the particles which come from the source, without having to simulate the background particles. The volumetric micro-mixing model uses the IEM – Interaction by Exchange with the Mean micro-mixing equation, which is simpler than the IECM model:

$$\frac{dC}{dt} = -\frac{C - \bar{c}}{\tau_m} \tag{4}$$

because simulating only the particles coming from the source does not allow to correctly sample all directions of the flow to calculate the conditional mean. The mean concentration $\bar{c}$ is calculated by the macro-mixing model:

$$\bar{c} = \frac{1}{V_{cell}} \sum_{i \in cell} m_i \quad (5)$$

where m_i is the mass of pollutant carried by each particle i that is in the control volume V_{cell}. In the volumetric micro-mixing approach, Cassiani (2013) proposes to calculate a volume V_i associated with each particle, defined from m_i and C_i by the relation:

$$V_i = \frac{m_i}{C_i} \quad (6)$$

By introducing equation 6 into equation 5, we obtain:

$$\bar{c} = \sum_{i \in cell} \frac{V_i}{V_{cell}} C_i = \sum_{i \in cell} f_i C_i \quad (7)$$

where $f_i = V_i / V_{cell}$ is interpreted as a frequency associated with the particle i and the concentration C_i. In this approach, the average concentration can be seen as the weighted average of the concentrations C_i of the particles coming from the source, of frequencies f_i on one hand, and of the zero concentrations of the particles not having passed through the source (implicit term equal to zero in this equation) on the other hand. By generalization, Cassiani (2013) proposed to calculate the n^{th} order ordinary moments by the same approach:

$$\overline{c^n} = \sum_{i \in cell} \frac{V_i}{V_{cell}} C_i^n \quad (8)$$

The volumetric micro-mixing model of Cassiani was tested by Marro et al. (2018). These authors showed that the volumetric approach gave satisfactory results for the variance of the fluctuations but poor results for the moments of higher order. To overcome this limitation, Marro et al. (2018) proposed to calculate the higher order moments from the mean and the variance, assuming that the PDF of the distribution follows a Gamma law, as it is frequently observed in the literature (Cassiani et al., 2020).

Even if it gives results which seem satisfactory on the configurations tested, the volumetric micro-mixing model of Cassiani introduces a volume and a probability frequency, associated with each particle, which are not fully satisfactory. Indeed, assuming that the mass of pollutant transported by each particle remains unchanged (in the absence of chemical, radioactive and deposition processes), equation 6 suggests that the volume of each particle is inversely proportional to its concentration, as if the concentration would evolve not by diffusion but by a compressibility effect, which has obviously no sense. The concentration of a particle varies by diffusive transfer to other particles, without variation in its volume.

The notion of probability frequency, which would be different for each particle and function of its concentration, is also questionable. First of all, all the particles rejected at the emission are equiprobable and there is no reason for this equiprobability to be modified during the transport of the particles. Furthermore, the calculated probability f_i being proportional to the volume V_i, the most probable particles would be the largest particles, having the lowest concentration. Obviously, this makes no sense. In reality, it is a mistake to interpret equation 7 as a weighted average, where f_i would be a frequency associated with each particle, and it is easy to show that there exists an infinite number of sequences f_i such that $\bar{c} = \sum_{i \in cell} f_i C_i$, for a given sequence of C_i. It is obvious that all these sequences cannot simultaneously represent the sequence of probabilities associated with the particles.

This is to avoid these conceptual limitations that a new approach was developed for the BUILD software, called " clipped distribution micro-mixing model".

Clipped distribution micro-mixing model

The micro-mixing model with clipped distribution adopts some ideas introduced in the volumetric approach of Cassiani (2013). The trajectories and the evolution of the concentration of particles from the source are simulated by the stochastic differential equation and by the IEM micro-mixing model. Particles that do not pass through the source are not simulated.

In the general case of an unsteady release, each particle emitted at the source is characterized by:

- a concentration C_i initialized to the concentration of the source C_s

$$C_i = C_s = \frac{Q_{m,specie}}{Q_{v,fluid}} \tag{9}$$

- a mass m_i

$$m_i = \frac{Q_{m,specie}\,\Delta t}{N_{part}} \tag{10}$$

where $Q_{m,specie_i}$ is the instantaneous mass emission rate of pollutant and $Q_{v,fluid}$ the instantaneous volume rate of fluid at the source, at the instant of emission of the particle. N_{part} is the number of particles emitted at the same time, during the time step Δt. The mass m_i can possibly change during the transport of particles under the effect of chemical or radioactive transformations or under the effect of deposition.

- a volume V_i

$$V_i = \frac{Q_{v,fluid}\,\Delta t}{N_{part}} \tag{11}$$

Note that in the present model, the volume V_i associated with each particle is invariant, the flow being assumed to be incompressible.

The concentration of particles at the source is by definition the maximum concentration value in the domain. By dilution with the particles coming from the outside, the average concentration in the field will be lower than the concentration of the source so that under the effect of equation 4, the concentration of each particle emitted by the source will decrease in order to get closer to the average concentration. Symmetrically, the particles not passing through the source are transported from upstream of the source with a zero concentration and will see their concentration increase under the effect of the equation 4 to get closer to the average concentration.

Based on this observation, the main hypothesis made in the present approach consists of assuming that at any point in the flow, within a control volume V_{cell}, the $N_{part,cell}$ particles coming from the source sample the upper part of the concentration PDF, as shown on **Figure 2**.

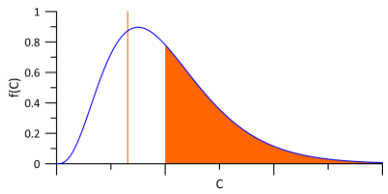


Figure 2. Illustration of the PDF of the concentration distribution and its clipped representation. The particles coming from the source correspond to the right part (in orange) of the distribution. Background particles are represented by a single concentration value (orange vertical line, left).

The fraction ϕ_{up} of the pdf resolved by the particles coming from the source corresponds to the fraction of the control volume V_{cell} occupied by these particles:

$$\phi_{up} = \frac{1}{V_{cell}} \sum_{i \in cell} V_i \tag{12}$$

We can show that $\phi_{up} = \bar{c}/C_s$, which can be interpreted as a dilution ratio of the mean concentration $\bar{c}$ relative to the source concentration C_s. Each of the $N_{part,cell}$ particles present in the cell is equiprobable, with frequency f:

$$f = \frac{\phi_{up}}{N_{part,cell}} \tag{13}$$

The second hypothesis of the model consists of representing the concentration of all the background particles (not having passed through the source) present in the cell by a single concentration value denoted C_{low} (illustrated by the orange vertical line on the **Figure 2**). The sum of the probabilities being equal to 1, the probability ϕ_{low} associated with the concentration C_{low} is such that:

$$\phi_{low} = 1 - \phi_{up} \tag{14}$$

The concentration distribution described previously, consisting of the $N_{part,cell}$ values C_i of frequency f and the concentration C_{low} of probability ϕ_{low} is called "clipped distribution".

Writing the average concentration from this distribution gives the relationship:

$$\bar{c} = (1 - \phi_{up})C_{low} + \sum_{i \in cell} f C_i \quad (15)$$

This relationship allows to determine the value of C_{low} from the known parameters:

$$C_{low} = \frac{\bar{c} - \sum_{i \in cell} f C_i}{1 - \phi_{up}} \quad (16)$$

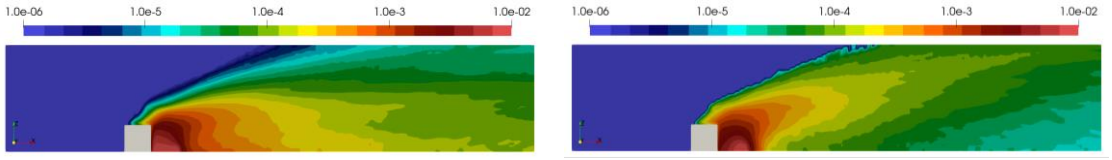
It then becomes possible to calculate the ordinary moments of higher orders, from the clipped distribution:

$$\overline{c^n} = (1 - \phi_{up})C_{low}^n + \sum_{i \in cell} f C_i^n \quad (17)$$

The previous modelling approach has been implemented in the BUILD operational Lagrangian dispersion model (Soulhac et al., 2022).

Model results and discussion

The clipped distribution micro-mixing model has been evaluated on theoretical test cases (ability to reproduce the Gamma distribution moments by the clipped distribution) and on experimental databases (point source in turbulent boundary layer on flat terrain, isolated 2D obstacle). **Figure 3** illustrates $\bar{c}$ and σ_c field in the wake of a 2D obstacle.



Mean concentration $\bar{c}$ Concentration standard deviation σ_c

Figure 3. Application of the clipped distribution micro-mixing model to simulate concentration fluctuations around an isolated 2D obstacle.

The results demonstrate the ability of the model to reproduce the fluctuation characteristics, without significant additional computational cost compared with a macro-mixing Lagrangian model.

CONCLUSION

In this work, a new model is proposed to describe concentration fluctuations in the BUILD operational Lagrangian dispersion model. The model is an improved version of the volumetric micro-mixing model of Cassiani (2013), based on the assumption of a clipped PDF distribution where the particles advected from the source sample the upper part of the distribution. This approach proves to be theoretically consistent, to have satisfactory validation results and to be numerically efficient for operational applications.

REFERENCES

Cassiani, M., Franzese, P., and Giostra, U., 2005. A PDF micromixing model of dispersion for atmospheric flow. Part I : development of the model, application to homogeneous turbulence and to neutral boundary layer. *Atmospheric Environment*, **39** (8), 1457–1469.

Cassiani, M., 2013. The Volumetric Particle Approach for Concentration Fluctuations and Chemical Reactions in Lagrangian Particle and Particle-grid Models. *Bound. Layer Meteor.*, **146** (2), 207–233.

Cassiani, M., Bertagni, M. B., Marro, M., and Salizzoni, P., 2020. Concentration Fluctuations from Localized Atmospheric Releases. *Bound. Layer Meteor.*, **177**, 461–510.

Marro, M., Salizzoni, P., Soulhac, L., and Cassiani, M., 2018. Dispersion of a Passive Scalar Fluctuating Plume in a Turbulent Boundary Layer. Part III : Stochastic Modelling. *Bound. Layer Meteor.*, **167** (3), 349–369.

Pope, S. B., 1998. The vanishing effect of molecular diffusivity on turbulent dispersion : implications for turbulent mixing and the scalar flux. *Journal of Fluid Mechanics*, **359**, 299–312.

Postma, J. V., Wilson, J. D., and Yee, E., 2011. Comparing Two Implementations of a Micromixing Model. Part I : Wall Shear-Layer Flow. *Bound. Layer Meteor.*, **140** (2), 207–224.

Soulhac, L., Lamaison, G., Charvolin, P., Nguyen C. V., Slimani, M., and Armand, P., 2022. Development and validation of the BUILD operational dispersion model for accidental or deliberate releases in complex area. Harmo21. Conf., Aveiro, Portugal.