Adaptation of the Lagrangian module of a CFD code for atmospheric dispersion of pollutants in complex urban geometries and comparison with existing Eulerian results

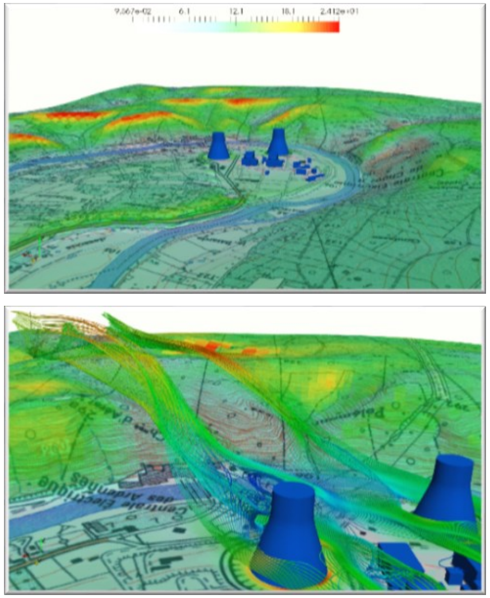
Meissam Bahlali, E. Dupont, B. Carissimo
CEREA – EDF R&D, Chatou, France

October 11, 2017
HARMO18, Bologna, Italy

CONTENTS

CONTENTS

CONTEXT AND OBJECTIVES



Source:
R. Bresson, EDF R&D

- Context:
  - Turbulent dispersion = **advection** + **turbulent diffusion**.
    - wide range of eddies in the atmospheric boundary layer which all participate in their own way to the transport and diffusion of the cloud
    - in particular: turbulent dispersion is not as effective **close to the emission source** as opposed to **further away** ➔ need to correctly model the effect of the different turbulent structures.
  - Multiple families of models: **Gaussian**, **Eulerian** (SGDH, GGDH, AFM, DFM…), **Lagrangian** models…

- Objectives:
  - To adapt of the **Lagrangian stochastic model** of the CFD code ***Code_Saturne*** in order to simulate **near-field dispersion of pollutants** in complex environments including buildings and taking into account atmospheric stratification.
  - To complete the existing Eulerian modelling of these phenomena → **compare and clarify the differences between the approaches, making use of the same CFD code**.

CONTENTS

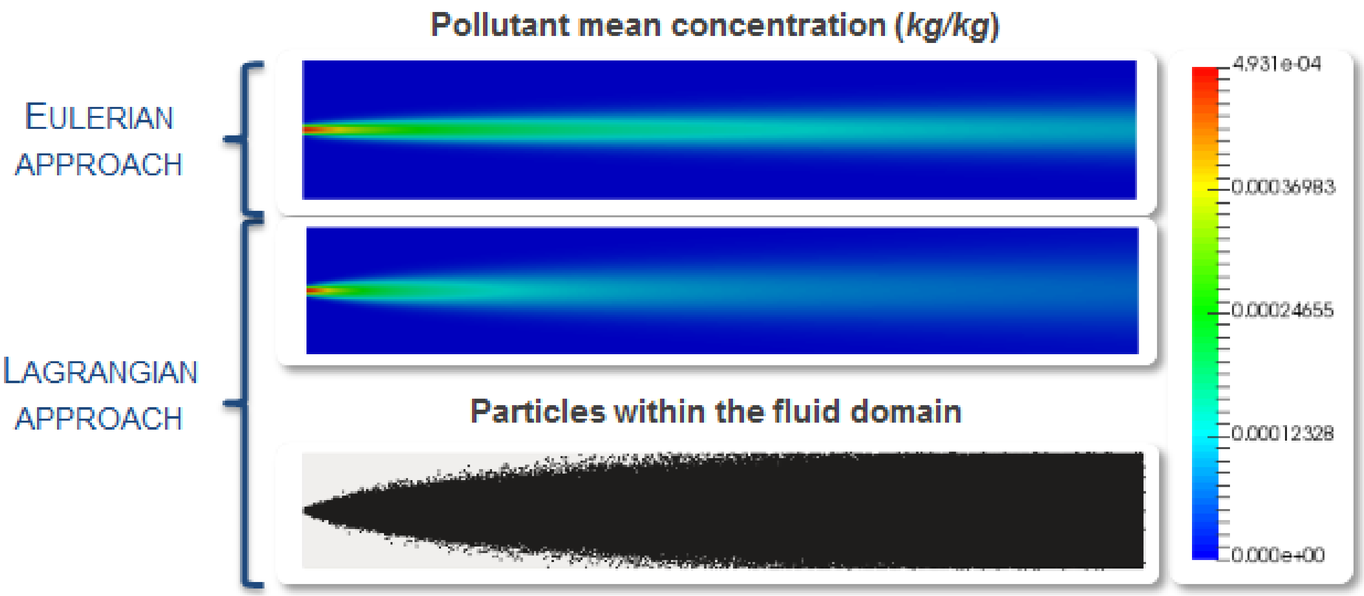
PRESENTATION OF THE APPROACH

- Calculation of the flow field (*"continuous phase"*): **mean Navier-Stokes equations**

$$\begin{cases} \dfrac{\partial \bar{\rho}}{\partial t} + \dfrac{\partial (\bar{\rho}\widetilde{u}_i)}{\partial t} = 0 \\ \dfrac{\partial (\bar{\rho}\widetilde{u}_i)}{\partial t} + \dfrac{\partial (\bar{\rho}\widetilde{u}_i\widetilde{u}_j)}{\partial x_j} = -\dfrac{\partial \bar{p}}{\partial x_i} + \dfrac{\partial}{\partial x_i}\left(\overline{\tau_{ij}} - \bar{\rho}\overline{u'_i u'_j}\right) - \bar{\rho} g \delta_{iz} \end{cases}$$

- Calculation of the dispersion of the pollutants within this flow field (*"dispersed phase"):* 2 main types of models
  - **Eulerian/Eulerian** models
  - **Eulerian/Lagrangian** models

EULERIAN AND LAGRANGIAN APPROACHES



EULERIAN APPROACH

- Mean advection-diffusion equation for a scalar *c*:

$$\frac{\partial \bar{c}}{\partial t} + \bar{u}_j \frac{\partial \bar{c}}{\partial x_j} = \frac{\partial}{\partial x_j}\left(D \frac{\partial \bar{c}}{\partial x_j} - \overline{u_j' c}\right) + \bar{S} + \bar{R}$$

- Velocity and turbulence fields → solved by the CFD code *Code_Saturne* using RANS models with classical k-ε or R_{ij}-ε closures adapted to the atmosphere and complex geometries

→ *APPROACH THAT HAS BEEN USED AT EDF R&D SO FAR.*

LAGRANGIAN APPROACH

- Particle's equation of motion:

$$\rho_p \frac{\pi D_p^3}{6} \frac{d\mathbf{U}_p}{dt} = \underbrace{\rho_p \frac{\pi D_p^3}{6} \frac{\mathbf{U}_s - \mathbf{U}_p}{\tau_p}}_{\text{Drag force}} + \underbrace{\frac{\pi D_p^3}{6}(\rho_p - \rho)\mathbf{g}}_{\text{Buoyancy force}} + \underbrace{\mathbf{F}_{ma}}_{\text{Added mass force}} + \underbrace{\mathbf{F}_{gp}}_{\text{Pressure-gradient force}} + \underbrace{\mathbf{F}_h}_{\text{History (or Basset) term}}$$

where: $\mathrm{U}_s(t) = \mathrm{U}_f(\mathrm{X}(t),t)$ is the velocity of the fluid sampled through the trajectory of the particle

WHY USE A LAGRANGIAN MODEL?

- **Diffusion theory** [Taylor, 1921] ➔ if we consider particle dispersion from a point source in stationary isotropic turbulence, there are 2 different regimes of diffusion:

$$\sigma_y^2(t) = 2\sigma_{U_{f,x}}^2 \int_0^t (t-s) R_{L,x}(s)\,\mathrm{d}s$$

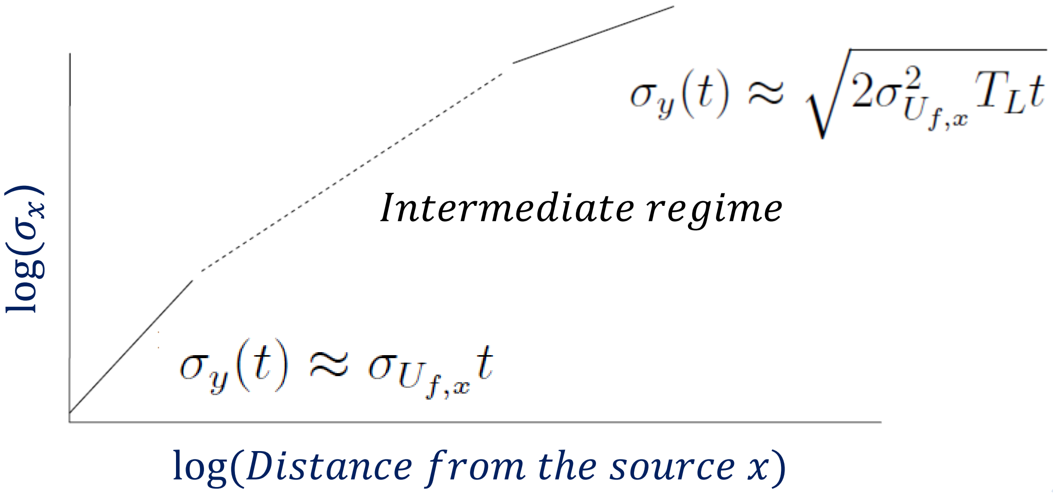
  - **Near-field ($t << T_L$):**

    $$\sigma_y(t) \approx \sigma_{U_{f,x}} t$$

  - **Far-field ($t >> T_L$):**

    $$\sigma_y(t) \approx \sqrt{2\sigma_{U_{f,x}}^2 T_L t}$$

Source: C. Seigneur, CEREA



WHY USE A LAGRANGIAN MODEL?

- **Eulerian approach** used at EDF R&D so far: **RANS with *k-ε* closure**. However: turbulent viscosity models imply **a turbulent diffusivity *K* independent from the distance to the source** and:

$$\sigma_y(t) = \sqrt{2Kt} \qquad \text{where:} \quad K = C_\mu \frac{k^2}{\epsilon}$$

$\propto \sqrt{t}$

⇒ Far-field modelling

→ **This model is unable to reproduce near-field behaviour.**

- **Lagrangian approach with Langevin model** yields [Pope, 2001]:

$$R_L(s) = exp(-|s|/T_L)$$

hence:

$$\sigma_y^2(t) = 2\sigma_{U_{f,x}}^2 T_L[t - T_L(1 - e^{-t/T_L})]$$

Near-field

$t << T_L$

$$\sigma_y(t) \approx \sigma_{U_{f,x}} t$$

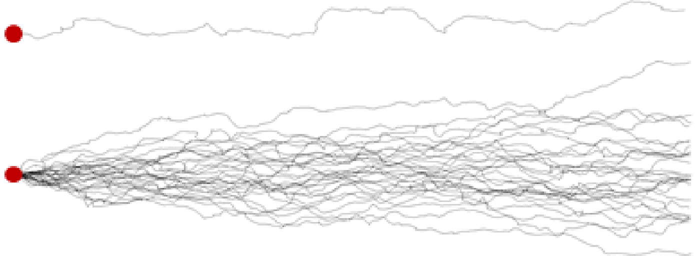
$t >> T_L$

Far-field

$$\sigma_y(t) \approx \sqrt{2\sigma_{U_{f,x}}^2 T_L t}$$

→ **This model does discriminate the two different diffusion regimes.** Note that: an Eulerian RANS model not based on turbulent viscosity approx. but with a **complete transport of turbulent scalar fluxes (*“DFM”*)** would also have this property ➔ work in progress.

TO SUM UP…



Source: RECORD report (ECL)

Particles' displacement within a turbulent flow

- Equation of motion solved for each particle:

$$\boxed{\rho_p \frac{\pi D_p^3}{6}\frac{d\mathbf{U}_p}{dt} = \rho_p \frac{\pi D_p^3}{6}\frac{\mathbf{U}_s - \mathbf{U}_p}{\tau_p} + \frac{\pi D_p^3}{6}(\rho_p - \rho)\mathbf{g} + \mathbf{F}_{ma} + \mathbf{F}_{gp} + \mathbf{F}_h}$$

where: $\mathrm{U_s}(t) = \mathrm{U_f}(\mathrm{X}(t),t)$ is the velocity of the fluid sampled through the trajectory of the particle

➔ This equation needs closure. Indeed: $\mathbf{U_s}(t) = \mathbf{U_f}(\mathbf{X}(t), t) = ?$

- *Code_Saturne* with **RANS models** only provides: $< \mathbf{U_f}(\mathbf{X}(t), t) >$

➔ *PDF (PROBABILITY DENSITY FUNCTION) METHODS*:

development of a Lagrangian stochastic model to reconstruct the turbulence effects

CONTENTS

MODEL FOR U$_S$: *SIMPLE LANGEVIN MODEL*

[POPE, 2001]

$$\left\{\begin{aligned} dX_i &= U_{p,i}(t)dt \\ dU_{p,i} &= \frac{U_{s,i}-U_{p,i}}{\tau_p}dt + g_i dt \\ dU_{s,i}(t) &= a_i(\mathbf{X}(t),\mathbf{U}_s(t),t)dt + \textstyle\sum_j b_{ij}(\mathbf{X}(t),\mathbf{U}_s(t),t)dW_j \end{aligned}\right.$$

Heavy particles hypothesis

Limit case of fluid particles: $\tau_p \rightarrow 0$

Simple Langevin Model

$$\boxed{dU_{s,i} = \underbrace{-\frac{1}{\rho}\frac{\partial \overline{P}}{\partial x_i}dt - \frac{U_{s,i}-\overline{U_{f,i}}}{T^*_{L,i}}dt}_{a_i\,dt} + \underbrace{\sqrt{C_0\overline{\epsilon}}dW_i}_{b_{ij}}}$$

Where: $T^*_{L,i} = \dfrac{T_{L,i}}{1+\beta\frac{|\mathbf{U}_f-\mathbf{U}_p|}{\sqrt{\frac{2}{3}k}}}$ and $\beta = \dfrac{T_{L,i}}{T_{E,i}}$ and $T_{L,i} = \dfrac{1}{\frac{1}{2}+\frac{3}{4}C_0}\dfrac{k}{\epsilon}$

MODEL FOR U_s: OTHER MODELS…

- Let us consider, for the sake of simplicity, the case of fluid particles: $\mathbf{U_s} = \mathbf{U_p}$
- 2 ways of modelling the evolution of the velocity field:
  - Through the instantaneous velocity $\mathbf{U_p}$
  - Through the fluctuating velocity $\mathbf{U_p}' = \mathbf{U_p} - <\mathbf{U_f}> \Rightarrow d\mathbf{U}'_\mathbf{p} = d\mathbf{U_p} - \overbrace{d<\mathbf{U_f}>}^{\textit{Obtained using Navier-Stokes eq.}}$

Model using:	Formulation
Instantateous velocity	$dU_{p,i} = -\frac{1}{\rho}\frac{\partial \overline{P}}{\partial x_i}dt - \frac{U'_{p,i}}{T_{L,i}}dt + \sqrt{C_0\overline{\epsilon}}dW_i$
Fluctuating velocity	$dU'_{p,i} = \left(\frac{\partial \overline{U'_{f,i}U'_{f,j}}}{\partial x_j} - U'_{p,j}\frac{\partial \overline{U_{f,i}}}{\partial x_j}\right)dt - \frac{U'_{p,i}}{T_{L,i}}dt + \sqrt{C_0\overline{\epsilon}}dW_i$

[Minier, Chibbaro, Pope, 2014]

MODEL FOR U_s: OTHER MODELS…

Model using:	Formulation
Instantateous velocity	$dU_{p,i} = -\frac{1}{\rho}\frac{\partial \overline{P}}{\partial x_i}dt - \frac{U'_{p,i}}{T_{L,i}}dt + \sqrt{C_0\overline{\epsilon}}dW_i$
Fluctuating velocity	$dU'_{p,i} = \left(\frac{\partial \overline{U'_{f,i}U'_{f,j}}}{\partial x_j} - U'_{p,j}\frac{\partial \overline{U_{f,i}}}{\partial x_j}\right)dt - \frac{U'_{p,i}}{T_{L,i}}dt + \sqrt{C_0\overline{\epsilon}}dW_i$

- **Example:** [Thomson, 1987] model ➔ $dU^{'}_{p,i} = a_i dt + b_{ij}dW_i$ where:

$$a_i = -\frac{C_0\epsilon}{2}\delta_{ij}\Gamma_{jk}U'_{p,k} + \frac{\Phi_i}{g_a}$$

and

$$\frac{\Phi_i}{g_a} = \overline{U_{f,l}}\frac{\partial \overline{U_{f,i}}}{\partial x_l} + \frac{\partial \overline{U_{f,i}}}{\partial x_j}(U_{p,j} - \overline{U_{f,j}}) + \frac{1}{2}\frac{\partial \tau_{il}}{\partial x_l} + \frac{1}{2}\overline{U_{f,m}}\frac{\partial \tau_{il}}{\partial x_m}\Gamma_{lj}(U_{p,j} - \overline{U_{f,j}}) + \frac{1}{2}\frac{\partial \tau_{il}}{\partial x_k}\Gamma_{lj}(U_{p,j} - \overline{U_{f,j}})(U_{p,k} - \overline{U_{f,k}})$$

- *Gaussian turbulence hypothesis*
- *Complicated formulation*

$$b_{ij} = \sqrt{C_0\epsilon}\delta_{ij}$$

- *Instantateous velocity:* pressure-gradient term clearly visible
- *Fluctuating velocity:* term hidden behind $\left(\frac{\partial \overline{U'_{f,i}U'_{f,j}}}{\partial x_j} - U'_{p,j}\frac{\partial \overline{U_{f,i}}}{\partial x_j}\right)dt$.

MODEL FOR U_s: OTHER MODELS…

WHY ARE WE CONCERNED ABOUT THE PRESENCE OF THE PRESSURE-GRADIENT TERM IN OUR MODELS?

- Well-mixed condition problem: *an initially uniform particle concentration in a turbulent flow should remain uniform*
    - ➔ condition that any Lagrangian stochastic model needs to meet
    - ➔ consistency with the mean Navier-Stokes equations
- [Minier, Chibbaro, Pope, 2014] : if the pressure-gradient term does not appear in the formulation of the model, then the well-mixed condition may not be fulfilled
- Note: need of full pressure field.

OUR REASONS FOR GOING FURTHER WITH THE *SIMPLE LANGEVIN MODEL* OF [POPE, 2001]

$$dU_{s,i} = \underbrace{-\frac{1}{\rho}\frac{\partial \overline{P}}{\partial x_i}dt - \frac{U_{s,i} - \overline{U_{f,i}}}{T^*_{L,i}}dt}_{a_i\, dt} + \underbrace{\sqrt{C_0 \bar{\epsilon}} dW_i}_{b_{ij}}$$

- It has a very **simple form** and the pressure-gradient term is clearly visible
- It is rigorous as it ensures **full consistency with the mean Navier-Stokes and the Reynolds equations (R_{ij}-ε) with Rotta's closure**
- **No hypothesis is made on the PDF of the velocity of the particles**
- To our knowledge, **it has not previously been used in the context of atmospheric dispersion**

OUR REASONS FOR GOING FURTHER WITH THE *SIMPLE LANGEVIN MODEL* OF [POPE, 2001]

$$dU_{s,i} = \underbrace{-\frac{1}{\rho}\frac{\partial \overline{P}}{\partial x_i}dt - \frac{U_{s,i} - \overline{U_{f,i}}}{T^*_{L,i}}dt}_{a_i\, dt} + \underbrace{\sqrt{C_0\bar{\epsilon}}dW_i}_{b_{ij}}$$

(1)

- It has a very **simple form** and the pressure-gradient term is clearly visible

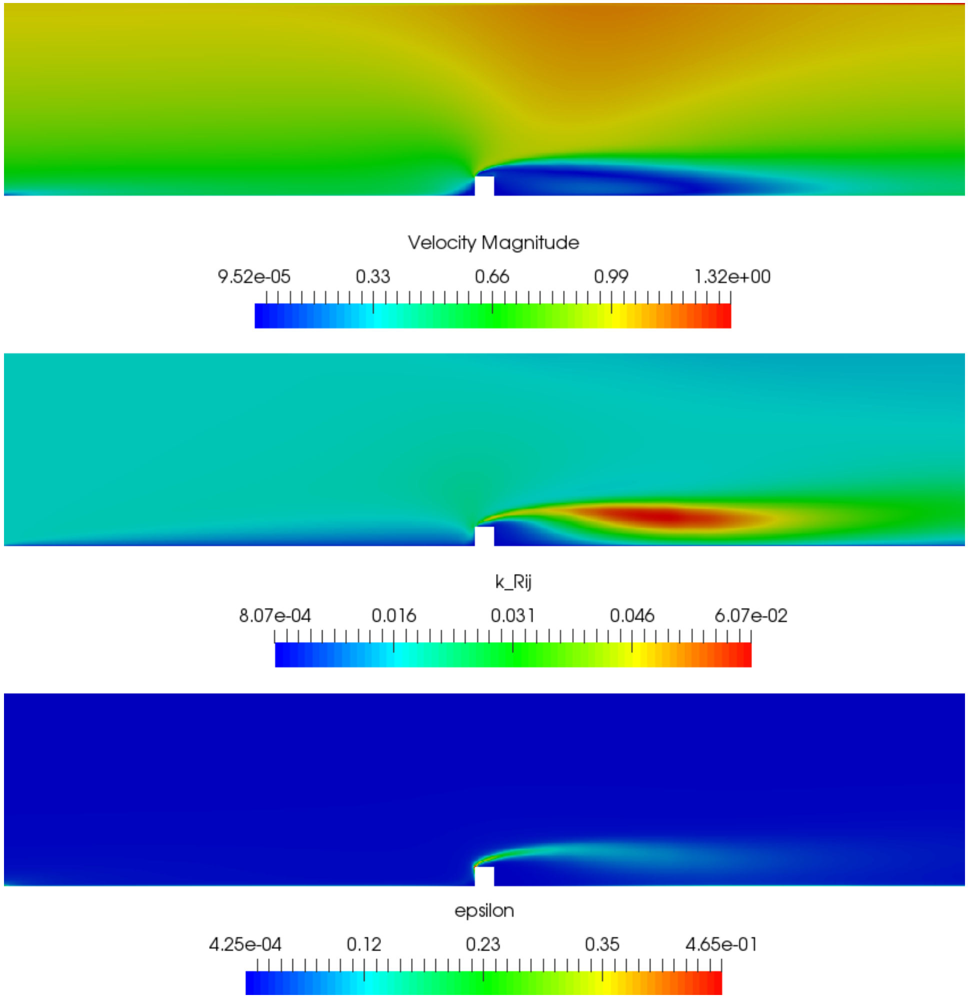
(2)

- It is rigorous as it ensures **full consistency with the mean Navier-Stokes and the Reynolds equations (R_{ij}-ε) with Rotta's closure**
- **No hypothesis is made on the PDF of the velocity of the particles**
- To our knowledge, **it has not previously been used in the context of atmospheric dispersion**

VALIDATION OF THE WELL-MIXED CRITERION WITH THE *SIMPLE LANGEVIN MODEL* OF [POPE, 2001]

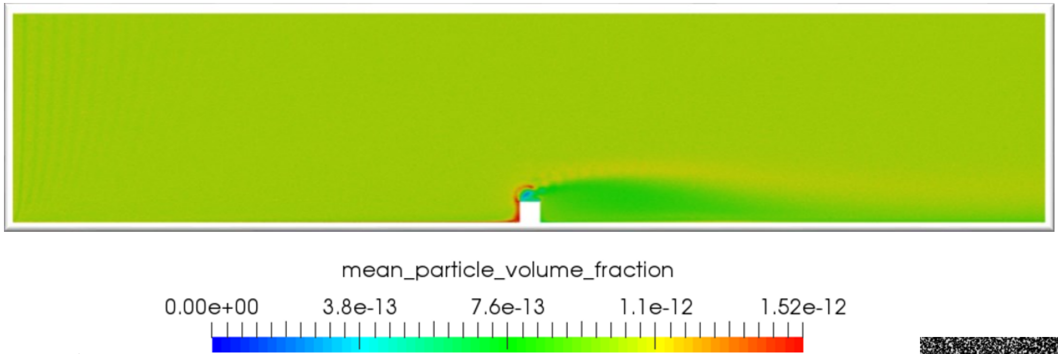
- **Inhomogeneous turbulence: obstacle within a boundary layer**

EULERIAN FLOW FIELD

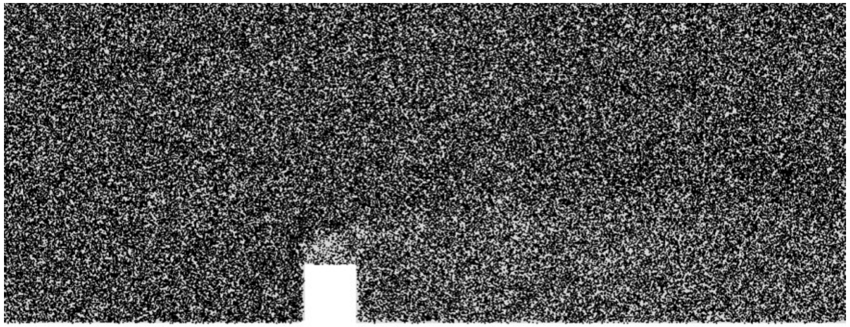


VALIDATION OF THE WELL-MIXED CRITERION WITH THE *SIMPLE LANGEVIN MODEL* OF [POPE, 2001]

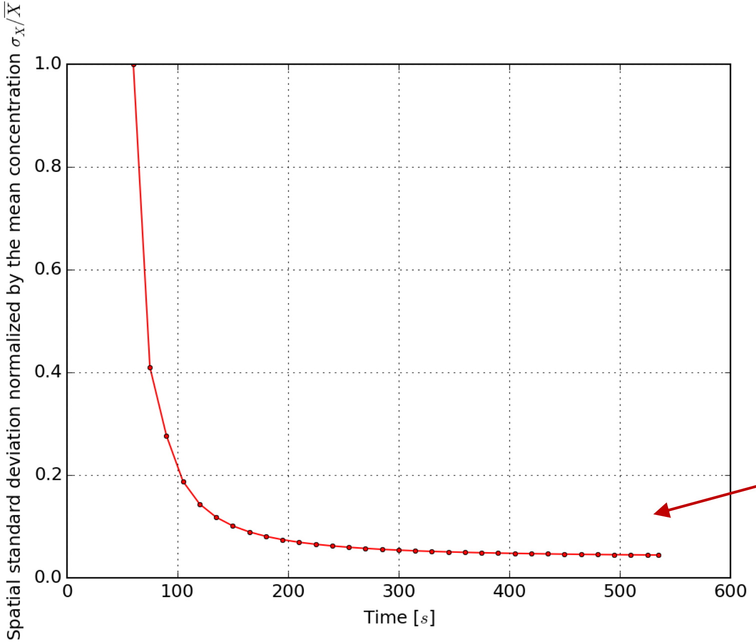
- **Inhomogeneous turbulence: obstacle within a boundary layer**



  - Example here with the ***R_{ij}-ε* model (Rotta's closure)**



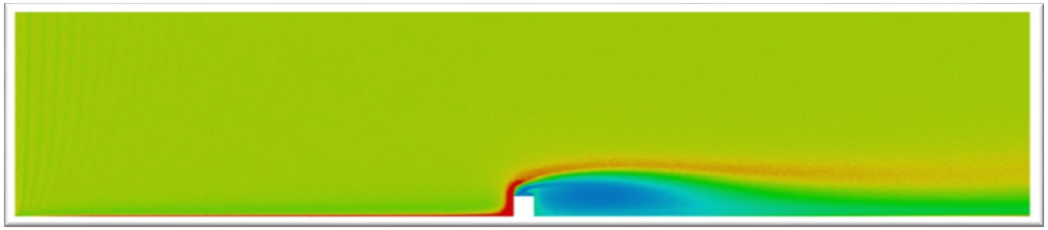
Particles within the fluid domain

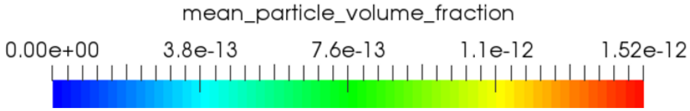


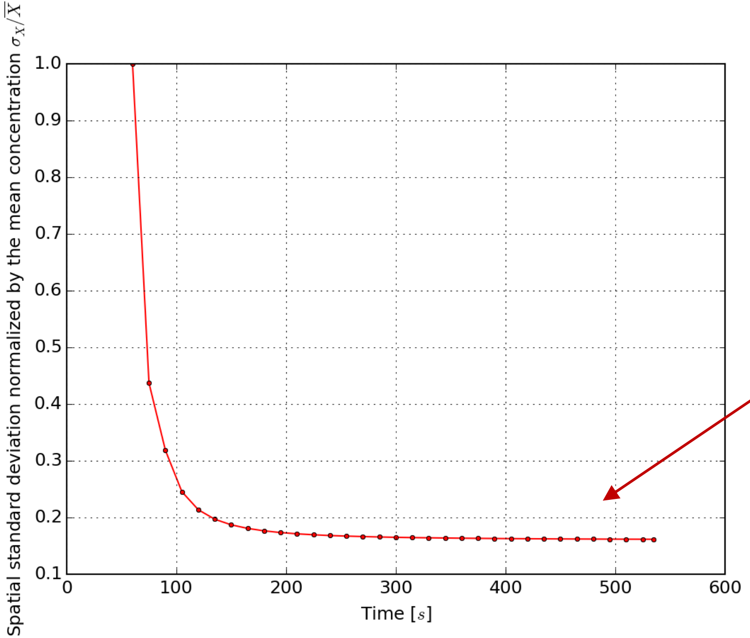
Spatial standard deviation normalized by the mean concentration: **≈ 4.4%**

VALIDATION OF THE WELL-MIXED CRITERION WITH THE *SIMPLE LANGEVIN MODEL* OF [POPE, 2001]

(1) What happens if we do not take into account the pressure-gradient term?

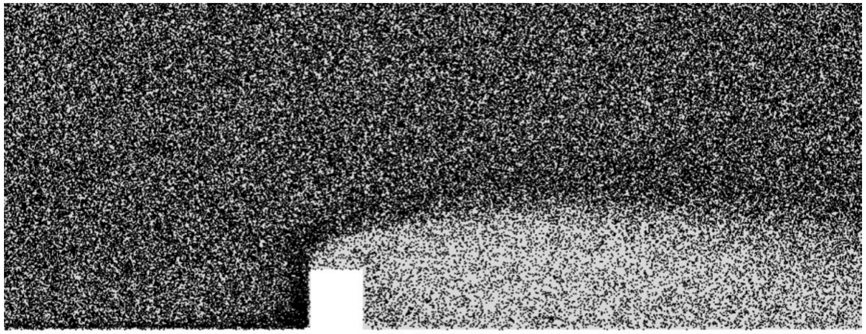






- Test performed here:

$$dU_{s,i} = -\cancelto{0}{\frac{1}{\rho}\frac{\partial \overline{P}}{\partial x_i}}dt - \frac{U_{s,i} - \overline{U_{f,i}}}{T^*_{L,i}}dt + \sqrt{C_0\overline{\epsilon}}dW_i$$



Particles within the fluid domain

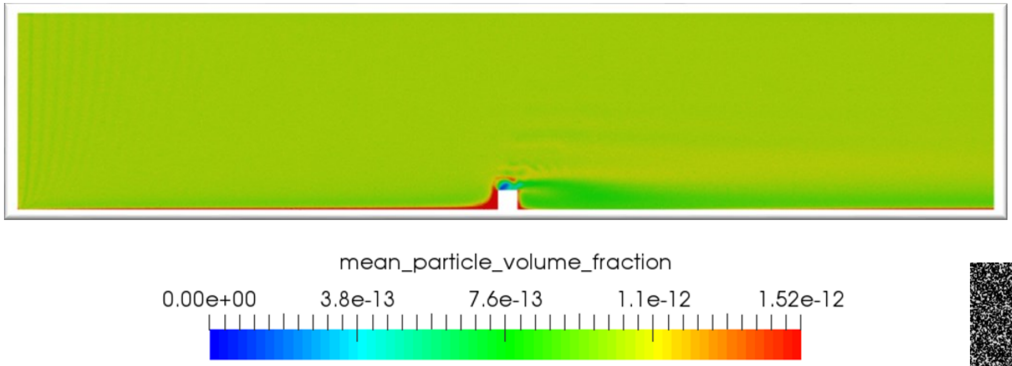
Spatial standard deviation normalized by the mean concentration: ≈ 16.2% > 4.4%!

ACCUMULATION OF PARTICLES

➔ SHOWS THE IMPORTANCE OF THE PRESSURE-GRADIENT TERM IN THE LANGEVIN EQUATION

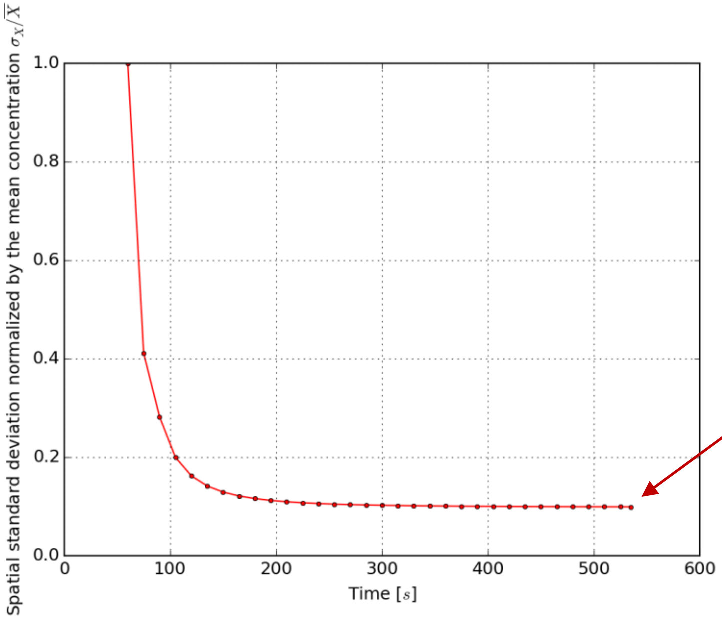
VALIDATION OF THE WELL-MIXED CRITERION WITH THE *SIMPLE LANGEVIN MODEL* OF [POPE, 2001]

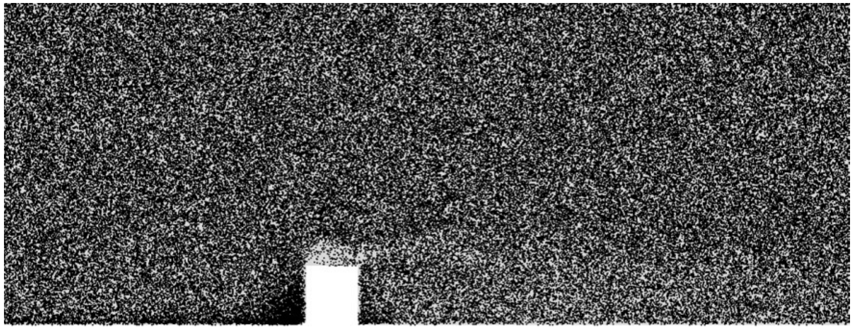
(2) What happens if the turbulence model used for the flow is not consistent with the SLM?



○ Model fully consistent with the SLM: ***R_{ij}-ε* model with Rotta's closure**

○ Example here with the ***k- ε* model**





Particles within the fluid domain

Spatial standard deviation normalized by the mean concentration: ≈ 9.9% >> 4.4%!

ACCUMULATION OF PARTICLES

➔ SHOWS THE IMPORTANCE OF MODELLING THE FLOW WITH A R_{IJ}-EPS MODEL (ROTTA'S CLOSURE)

CONTENTS

CALCULATION OF THE DISPERSED PHASE

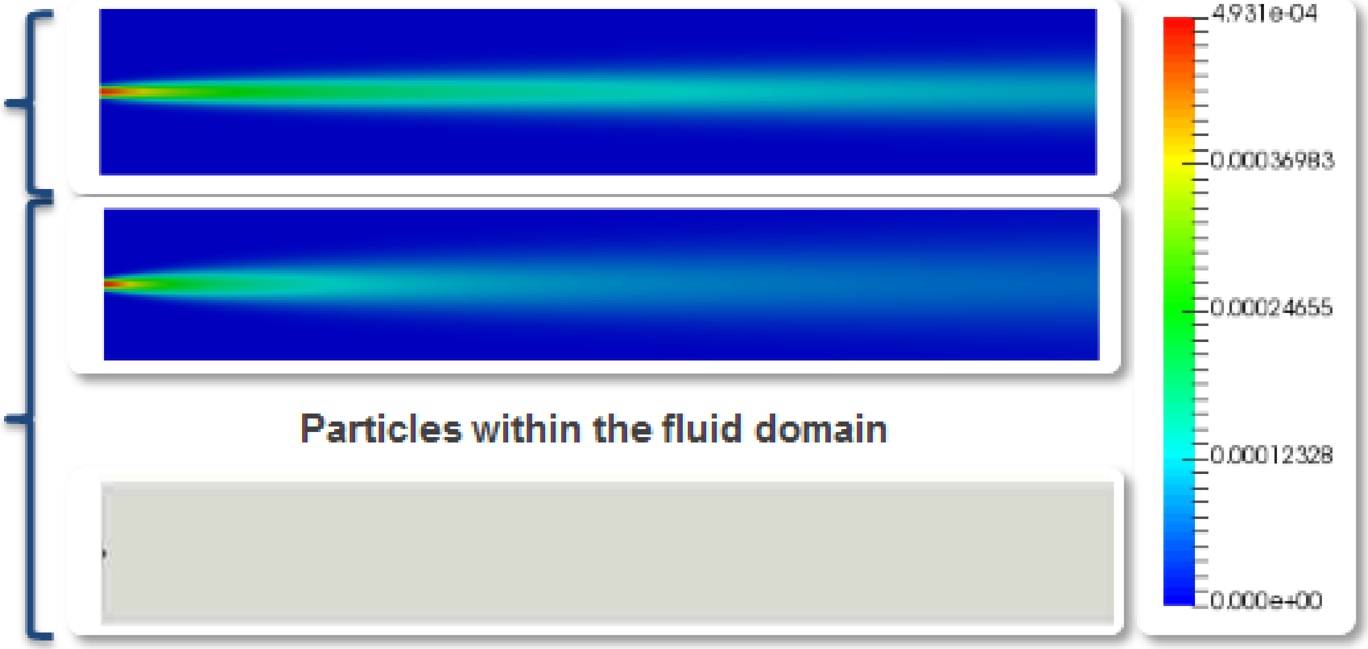
Taylor's analytical solution:

$$\frac{c}{Q} = \frac{1}{\sqrt{2\pi} U \sigma_x} \text{ with: } \sigma_x = \sqrt{\frac{2}{3}k}\,\frac{x}{U\sqrt{1+\frac{x}{2UT_L}}}$$

Pollutant mean concentration (*kg/kg*)

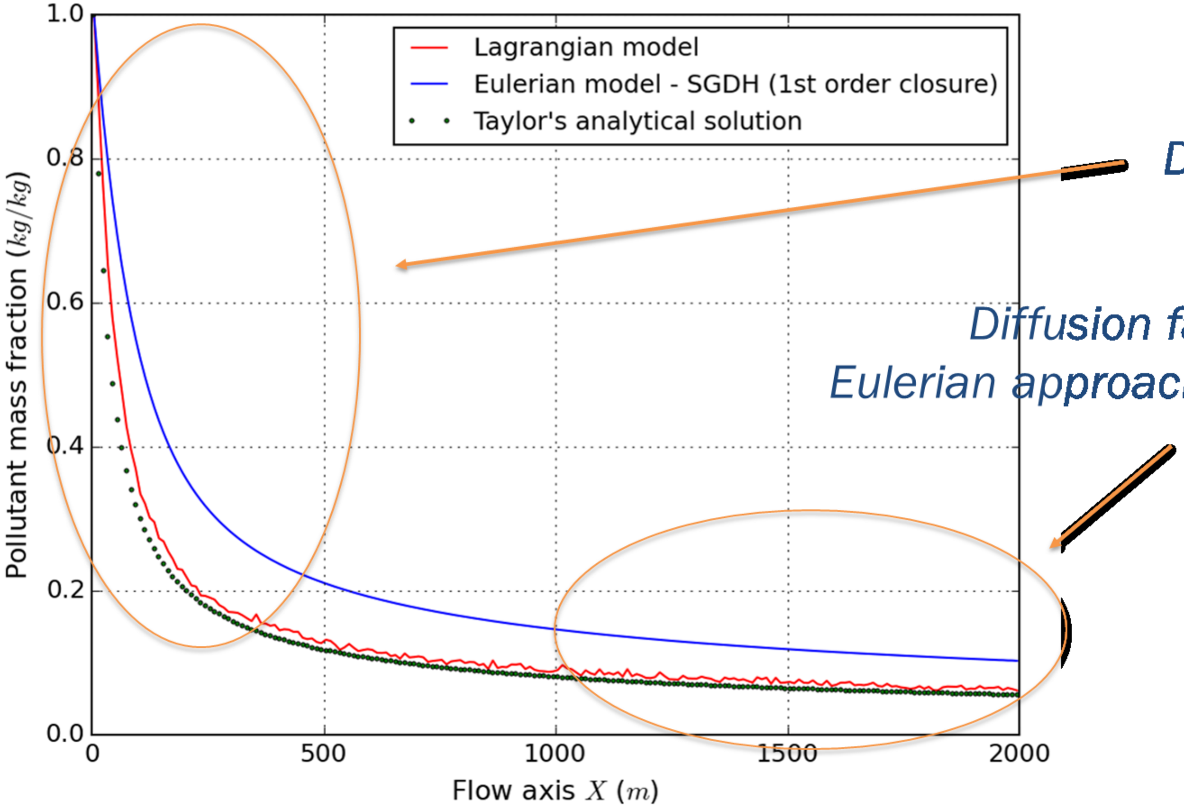
EULERIAN APPROACH

LAGRANGIAN APPROACH



Particles within the fluid domain

CALCULATION OF THE DISPERSED PHASE



Diffusion near the source

Diffusion far from the source
Eulerian approach ~ Lagrangian approach

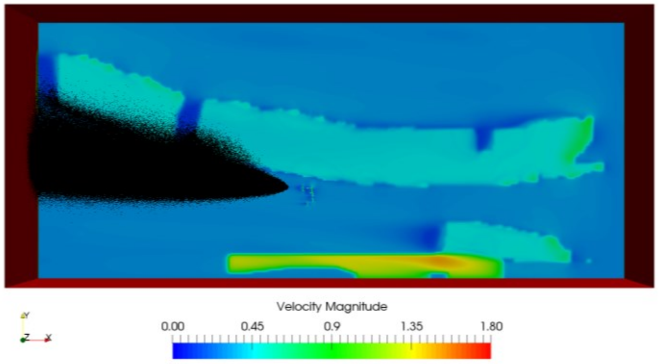
Maximum concentration (*kg/kg*) along the flow axis
Comparison of the two approaches

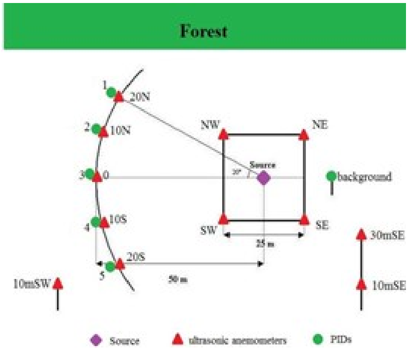
CONCLUSIONS AND PERSPECTIVES

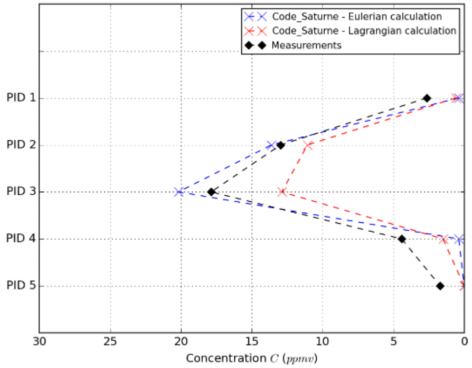
- Conclusions:
  - Objective: development of a **Lagrangian stochastic tool** to simulate **atmospheric dispersion simultaneously with Eulerian dispersion**
  - ***Simple Langevin Model*** of [Pope, 2001] : to our knowledge, never used in the context of atmospheric dispersion → yet, many advantages:
    - Pressure-gradient term included in an evident manner → *no spurious drifts*
    - Full consistency with the R_{ij}-*eps* model (Rotta's closure) → *careful when calculating the continuous phase!*
  - **Validation** of the **well-mixed criterion**: our model performs well, *even with an obstacle within a boundary layer*
  - **Validation** by checking with **analytical solution:** with our Lagrangian model, *distinction of the two regimes of diffusion*

CONCLUSIONS AND PERSPECTIVES

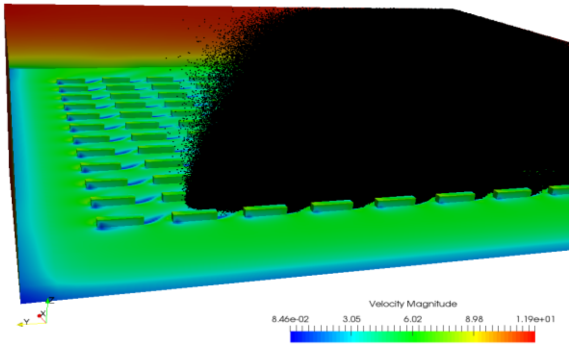
- Perspectives:
  - ☐ **Validation** on **SIRTA campaign** with R_{ij}-ε model (consistency issues between Navier-Stokes/Langevin eq.)

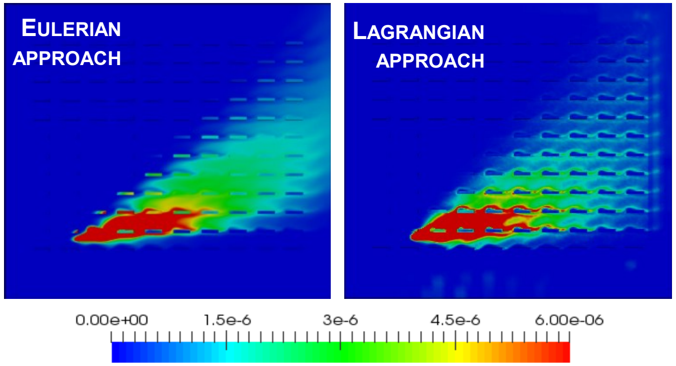






  - ☐ **Validation** on **MUST campaign** (Mock Urban Setting Test), Utah's desert, USA. Presence of obstacles.



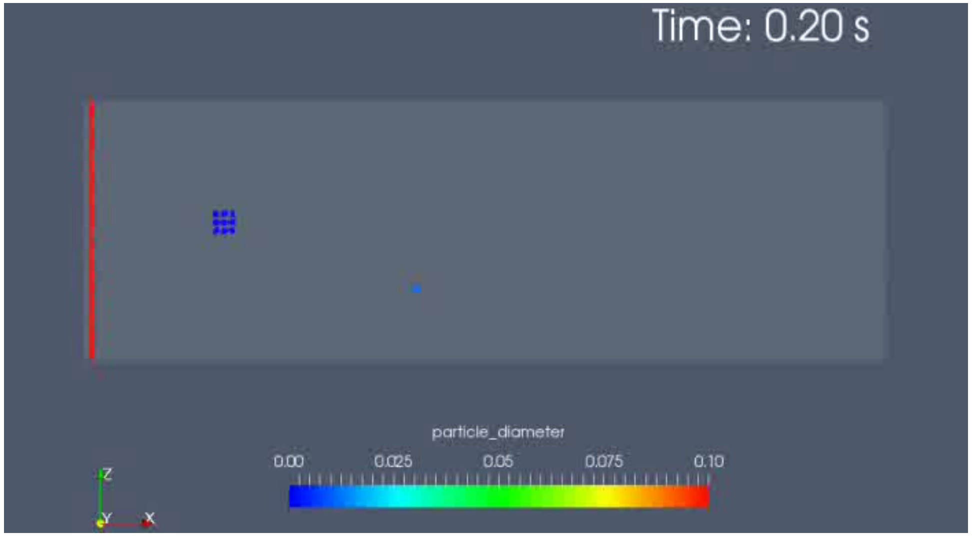


Preliminary results for case 2681829 (neutral conditions)

Other tested cases: 2681849 (neutral conditions), 2640246 (stable conditions)

  - ☐ R_{ij}-ε model with **DFM (*Differential Flux Model*)** for the scalars

THANK YOU FOR YOUR ATTENTION



References:

- Arya, S. P., 1999: Air pollution meteorology and dispersion (Vol. 6). Edition, New York: Oxford University Press.
- Minier, J.-P. et E. Peirano. 2001, *The PDF approach to turbulent polydispersed two-phase flows*, Physics Reports
- Minier, J.-P., S. Chibbaro et S. B. Pope. 2014, *Guidelines for the formulation of Lagrangian stochastic models for particle simulations of single-phase and dispersed two-phase turbulent flows*, Physics of Fluids
- Pope, S. B. 1994, *Lagrangian PDF methods for turbulent flows*, Annual review of fluid mechanics
- Pope, S. B. 2001, *Turbulent flows*
- Thomson, D. 1987, *Criteria for the selection of stochastic models of particle trajectories in turbulent flows*, Journal of Fluid Mechanics