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# On the Well-Mixed Condition and Consistency Issues in Hybrid Eulerian/Lagrangian Stochastic Models of Dispersion

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1 **On the well-mixed condition and consistency issues**  
2 **in hybrid Eulerian/Lagrangian stochastic models of**  
3 **dispersion**

4 **Meïssam L. Bahlali\*** · **Christophe**  
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8 **Abstract** We clarify issues related to the expression of Lagrangian stochastic  
9 models used for atmospheric dispersion applications. Two aspects are ad-  
10 dressed: the respect of the well-mixed criterion and the correspondence be-  
11 tween Eulerian and Lagrangian turbulence models when they are combined  
12 in practical simulations. In particular, it is recalled that the fulfillment of the  
13 well-mixed criterion depends only on the proper incorporation of the mean  
14 pressure-gradient term as the mean drift term of the Langevin equation. New  
15 consistency issues between duplicate fields within Eulerian/Lagrangian hy-  
16 brid formulations are also brought out, especially regarding turbulence mod-  
17 els, boundary conditions, and divergence-free condition. Such hybrid methods,  
18 where mean flow quantities calculated with an Eulerian approach are provided  
19 to the Lagrangian approach, are commonly used in atmospheric dispersion sim-  
20 ulations for their numerical efficiency. Nevertheless, it is shown that serious  
21 inconsistencies can result from coupling Eulerian and Lagrangian models that  
22 do not correspond to the same level of description of the fluid turbulence.

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**Table 1** List of abbreviations

CFD	Computational Fluid Dynamics	SDE	Stochastic Differential Equation
PDE	Partial Differential Equation	SLM	Simplified Langevin Model
PDF	Probability Density Function		

23 **Keywords** Dispersion models · Eulerian/Lagrangian methods · Stochastic  
 24 modeling · Turbulence · Well-mixed criterion

## 25 1 Introduction

26 Lagrangian stochastic models for atmospheric dispersion purposes have been  
 27 studied extensively since the 1980s. These models reproduce convective trans-  
 28 port in the atmosphere by explicitly tracking a large number of representative  
 29 fluid particles where, usually, the evolution of particle velocities is driven by a  
 30 stochastic differential equation of a Langevin type. Such equation includes two  
 31 terms, respectively known as the drift vector and the diffusion matrix, which  
 32 are to be determined. The diffusion matrix is defined following Kolmogorov’s  
 33 similarity theory and the main closure issue is therefore the expression of the  
 34 drift.

35 First well-known references in Lagrangian stochastic modeling are, for ex-  
 36 ample, Wilson et al. (1981); Sawford (1985); Van Dop et al. (1985); De Baas  
 37 et al. (1986), or the classic paper Thomson (1987). In most of these works,  
 38 the so-called ‘well-mixed condition’ issue was brought out as a challenging  
 39 issue. First introduced by Sawford (1986), this issue corresponds to the ther-  
 40 modynamic constraint stating that an initially uniform distribution of fluid  
 41 particles (each representing an equal amount of mass) in an incompressible  
 42 flow must remain uniform. The well-mixed criterion is a necessary criterion  
 43 for any Lagrangian stochastic model to be regarded as acceptable since its  
 44 violation means that density is no longer constant (therefore at variance with  
 45 the incompressibility constraint). For that reason, various authors have tried  
 46 to provide conditions to ensure that it is respected. It was shown by Sawford  
 47 and Guest (1988) and Borgas et al. (1997) that certain flow properties need  
 48 to be accounted for, see Wilson and Sawford (1996). Historically in the at-  
 49 mospheric literature, authors adopted other selection criteria and worked on  
 50 a case-by-case basis (homogeneous or inhomogeneous turbulence, Gaussian or  
 51 non-Gaussian turbulence hypothesis, convective, stable or neutral atmosphere,  
 52 etc.). As a result, a confusion surrounding expressions of the drift term in the  
 53 Langevin equation has sometimes led to non well-mixed models that made  
 54 various authors adopt a back-and-forth philosophy and add ad-hoc new terms  
 55 to make up for the problem (Lin and Gerbig 2013).

56 Since the works mentioned above, significant improvements in Lagrangian  
 57 stochastic modeling have been achieved in other fields where similar models  
 58 are currently applied, in particular in turbulent combustion modeling (Pope  
 59 1985, 1991), in single-phase flow turbulence modeling (Pope 1994b) as well as  
 60 in dispersed turbulent two-phase flows applications (Minier and Peirano 2001;

61 Minier 2015). For instance, Pope (1987) showed that a necessary and suffi-  
62 cient condition for the well-mixed criterion to be fulfilled is that the calculated  
63 mean velocity field satisfies the continuity equation and that this condition is,  
64 in turn, equivalent to incorporating properly the mean pressure gradient term  
65 in the Langevin model. However, in the recent atmospheric literature relative  
66 to Lagrangian dispersion modeling (see, e.g., Franzese (2003), Stohl et al.  
67 (2005), Alessandrini and Ferrero (2009), Tinarelli et al. (2013)), the formu-  
68 lations introduced by Pope and referred to as ‘probability density function  
69 (PDF) methods’ are not widely used. Cassiani et al. (2005a,b, 2007) referred  
70 to Pope’s PDF framework for micro-mixing modeling but followed Thomson  
71 (1987)’s approach to close the fluctuating pressure gradient and viscous terms.

72 In this context, the present study aims at bridging the developments made  
73 in Lagrangian stochastic models in reactive and two-phase flows with atmo-  
74 spheric dispersion applications. It has a two-fold objective: (a) to clarify re-  
75 maining confusions about the well-mixed condition; (b) to provide a better  
76 understanding of consistency issues between fields obtained from Eulerian and  
77 Lagrangian simulations when hybrid Eulerian/Lagrangian numerical formula-  
78 tions are used.

79 The paper is organized as follows: in Sect. 2, Lagrangian stochastic models  
80 for atmospheric dispersion are introduced and the formulation of the well-  
81 mixed condition, as well as consistencies between duplicate turbulence mod-  
82 els and wall-boundary conditions, are presented. To illustrate how consistent  
83 formulations can be developed in the context of hybrid Eulerian/Lagrangian  
84 frameworks, the details of such a model are briefly provided. Numerical assess-  
85 ment of the respect of the well-mixed criterion through the simple introduction  
86 of the mean pressure gradient is detailed in Sect. 3, through three simulations  
87 of non-homogeneous turbulent flows that cover a wide range of practical sit-  
88 uations. More specifically, numerical results obtained in three standard cases  
89 are used to illustrate two main points:

- 90 (i) The satisfaction of the well-mixed criterion depends only on the proper  
91 introduction of the mean pressure-gradient term as the mean drift compo-  
92 nent of the Langevin model, regardless of further details.
- 93 (ii) In so-called Eulerian/Lagrangian hybrid numerical formulations, such as  
94 that considered in present simulations, the mean fields corresponding to  
95 the first and second moments of the velocity field are duplicate fields and  
96 need to be regarded as such. In other words, identity between predictions  
97 of the Eulerian and Lagrangian solvers must be verified for a model and  
98 its numerical implementation to be acceptable.

## 99 **2 Particle Stochastic Methods: Theory and Numerics**

100 This section provides a brief description of the key concepts and issues be-  
101 hind particle stochastic methods. Interested readers are referred to existing  
102 comprehensive reviews for more details (Monin and Yaglom 1971; Pope 1985,  
103 1994a, 2000; Minier and Peirano 2001; Minier 2016).

**Table 2** Two existing formulations of the SLM

Model written in terms of:	Formulation
Instantaneous velocity	$dU_{p,i} = -\frac{1}{\rho_f} \frac{\partial \langle P_f \rangle}{\partial x_i} dt - \frac{U'_{p,i}}{T_L} dt + \sqrt{C_0 \epsilon_f} dW_i$
Fluctuating velocity	$dU'_{p,i} = \left( \frac{\partial \langle U'_{f,i} U'_{f,j} \rangle}{\partial x_j} - U'_{p,j} \frac{\partial \langle U_{f,i} \rangle}{\partial x_j} \right) dt - \frac{U'_{p,i}}{T_L} dt + \sqrt{C_0 \epsilon_f} dW_i$

## 104 2.1 The Simplified Langevin Model

105 A simplified Langevin model (SLM) is used (more details can be found in  
 106 Pope (1985, 2000); Minier and Peirano (2001)), with this Lagrangian stochastic  
 107 model describing the dynamics of (fluid) particles by explicitly tracking their  
 108 position  $X_p$  and velocity  $U_p$  according to,

$$dX_{p,i} = U_{p,i} dt, \quad (1a)$$

$$dU_{p,i} = -\frac{1}{\rho_f} \frac{\partial \langle P_f \rangle}{\partial x_i} dt - \frac{U_{p,i} - \langle U_{f,i} \rangle}{T_L} dt + \sqrt{C_0 \epsilon_f} dW_i. \quad (1b)$$

109 The first term on the right-hand side (r.h.s.) of Eq. 1b corresponds to the  
 110 mean pressure gradient (with  $\rho_f$  the fluid density and  $\langle P_f \rangle$  the mean pres-  
 111 sure of the fluid). In the second term on the r.h.s., the particle velocity re-  
 112 laxes toward the local mean fluid velocity taken at the particle location, i.e.  
 113  $\langle U_{f,i} \rangle = \langle U_{f,i} \rangle(t, \mathbf{X}_p(t))$ . The time scale for this relaxation is  $T_L$ , which rep-  
 114 represents the Lagrangian integral time scale  $T_L = \frac{k_f}{\epsilon_f} (\frac{1}{2} + \frac{3}{4} C_0)^{-1}$ . In the last  
 115 term,  $dW_j$  are independent Wiener processes,  $C_0$  a constant given by Kol-  
 116 mogorov's theory, and  $\epsilon_f$  the mean turbulence kinetic energy dissipation rate  
 117 at the particle position. It should be noted here that the simplified Langevin  
 118 model is appropriate to high Reynolds number and the effect of viscosity is  
 119 absent (Pope 2000). The viscous effect being of primary importance in the  
 120 viscous sublayer, additional terms are usually included in near-wall models  
 121 (see for example Sect. 2.2.2 or Waclawczyk et al. (2004) for near-wall viscos-  
 122 ity effects in Lagrangian PDF methods). Such models can be used for simple  
 123 boundary flows such as the channel flow (see Sect. 3.2) but are more problem-  
 124 atic in complex geometries as the flow behind an obstacle (see Sect. 3.3). The  
 125 viscous issues are still open and will be investigated in the future.

126 Another type of formulation for the SLM has been derived using the fluctu-  
 127 ating velocity  $U'_{p,i}$ , defined as  $U'_{p,i} = U_{p,i} - \langle U_{f,i} \rangle$ . The difference between  
 128 these two types of formulation for the SLM are summarized in Table 2 and  
 129 interested readers are referred to, e.g., Minier et al. (2014). It can be seen  
 130 that both formulations are similar (blue terms are identical) and there is no  
 131 intrinsic difference since a simple change of variables allows to go from one for-  
 132 mulation to the other. Yet, there are significant differences in the expression  
 133 of the mean pressure gradient: whereas it appears directly in the formulation  
 134 written with instantaneous velocities, it includes the derivative term of the

135 Reynolds-stress tensor in the formulation written with fluctuating velocities.  
136 We wish to emphasize here that ignoring this term results in spurious drift  
137 effects (see Minier et al. (2014) for more details). As a result, the proper ac-  
138 count of the mean pressure-gradient term is key in ensuring the well-mixed  
139 condition. In the following, only the formulation written with instantaneous  
140 velocities is considered.

## 141 2.2 Hybrid Eulerian/Lagrangian Simulations

142 In the following, we resort to a hybrid Eulerian/Lagrangian calculations where  
143 the fluid phase is simulated using an Eulerian solver and the particle phase is  
144 solved with a Lagrangian one. The use of such hybrid formulations requires  
145 a specific attention for the terms entering the particle dynamics, such as the  
146 mean fluid velocity at the particle location (see Eq. 1). In the following, the  
147 issues related to the consistency of the Eulerian and Lagrangian models are  
148 detailed.

### 149 2.2.1 Consistency Issues on Turbulence Models

150 If the proper introduction of the mean pressure gradient on the r.h.s. of Eq. 1  
151 is enough to ensure that the mean Navier–Stokes equation derived from the  
152 PDF model is correctly retrieved, the specific details of a Langevin model (i.e.,  
153 the last two terms on the r.h.s. of Eq. 1b) come into play when considering the  
154 second-order velocity moments or, in other words, the transport equations for  
155 the Reynolds-stress components. The connection between Lagrangian stochas-  
156 tic models was first developed in Pope (1994b) and has been addressed in de-  
157 tail in several works, cf. Pope (2000); Minier and Peirano (2001); Minier et al.  
158 (2014).

159 The derivation of the Reynolds-stress equations from a Langevin model,  
160 such as the SLM in Eq. 1, reveals that for each formulation of a Langevin  
161 model there is a corresponding second-order, or  $R_{ij} - \epsilon$ , turbulence model.  
162 This connection is of importance, first to indicate that Lagrangian stochastic  
163 are true second-order turbulence models when they are used as stand-alone  
164 approaches and, second, to point out a consistency issue when they are used  
165 in hybrid Eulerian/Lagrangian numerical formulations. In particular, an SLM  
166 for the Lagrangian solver is consistent with a Rotta second-order turbulence  
167 model for the Eulerian solver (with the Rotta constant deriving from the  
168 value taken from the  $C_0$  constant). More details are provided in Chibbaro and  
169 Minier (2011) and Minier (2015, 2016). It should be noted here that variants  
170 of the present hybrid Eulerian/Lagrangian formulation could be developed  
171 to match other models for the Eulerian solver (for instance using LES or  
172 Reynolds stress equation models). In that sense, the present formulation serves  
173 as an illustration of how consistent hybrid Euler/Lagrange formulations can  
174 be developed.

### 175 2.2.2 Consistency Issues on Boundary Conditions

176 Another issue is the formulation of wall-boundary conditions in particle stochastic  
 177 approaches, which is a subject that has received very little attention. For  
 178 instance, a first idea consists in applying specular rebound: every particle  
 179 that crosses a wall boundary and exits the computational domain is reflected  
 180 back with the same streamwise velocity component as the incoming one, i.e.  
 181  $U_{p,x}^{in} = U_{p,x}^{out}$  and  $U_{p,y}^{in} = U_{p,y}^{out}$ . Yet this amounts to writing a zero-flux bound-  
 182 ary condition for the streamwise velocity component, which fails to account for  
 183 the momentum exchange with the wall. Following the same spirit of the one  
 184 used to derive so-called wall-function boundary conditions in computational  
 185 fluid dynamics (CFD) codes, where a boundary condition is applied in the log-  
 186 arithmic region near the wall rather than at the wall itself (cf. Pope (2000)),  
 187 a better representation of wall-boundary conditions to capture the constant-  
 188 stress boundary layer is (assuming that  $z$  is the wall-normal direction)

$$U_{p,x}^{in} = U_{p,x}^{out} - 2 \frac{\langle U'_{f,x} U'_{f,z} \rangle}{\langle U'^2_{f,z} \rangle} U_{p,z}^{out} , \quad (2a)$$

$$U_{p,y}^{in} = U_{p,y}^{out} - 2 \frac{\langle U'_{f,y} U'_{f,z} \rangle}{\langle U'^2_{f,z} \rangle} U_{p,z}^{out} , \quad (2b)$$

$$U_{p,z}^{in} = -U_{p,z}^{out} , \quad (2c)$$

189 where the subscript ‘in’ stands for the particle’s incoming velocity value and  
 190 ‘out’ the outgoing one (see Fig. 1). The rationale behind these expressions for  
 191 particle-based stochastic models are detailed in Dreeben and Pope (1997) and  
 192 Minier and Pozorski (1999).

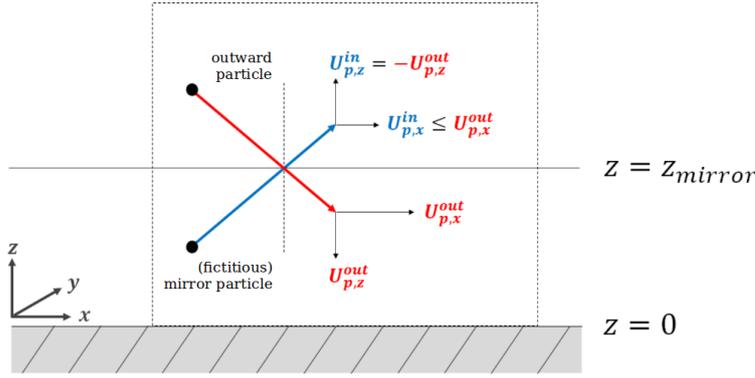
193 Such formulations are needed to reproduce the correct behavior of the mean  
 194 streamwise fluid velocity component in wall boundary layers. In hybrid Eulerian/  
 195 Lagrangian approaches, they also represent an additional consistency  
 196 issue since wall-boundary conditions are actually formulated twice, in the Eulerian  
 197 and in the Lagrangian solvers. Consistent wall-boundary conditions are  
 198 important for the correct computation of particle second-order moments near  
 199 walls as will be seen later in the case of an infinite channel flow (see Sect. 3.2).

### 200 2.2.3 Correction on particle velocities

201 In stand-alone approaches, the mean pressure is calculated as the constraint  
 202 needed to have  $\text{div}(\langle \mathbf{U}_p \rangle) = 0$  (cf. Minier and Pozorski (1999)). In hybrid  
 203 Eulerian/Lagrangian formulations, it is easier to use directly the mean pressure  
 204 gradient calculated by the Eulerian solver, say  $P^E$ , in the Langevin equations,  
 205 so that Eq. 1b can be expressed as

$$d\tilde{U}_{p,i} = -\frac{1}{\rho_f} \frac{\partial P^E}{\partial x_i} dt + dM_i , \quad (3)$$

206 where  $\langle dM_i \rangle = 0$ , and where the notation  $\tilde{U}_{p,i}$  is used to indicate that this is a  
 207 first estimation of particle velocities and where  $dM_i$  stands for the fluctuating



**Fig. 1** Sketch of the wall/particle interaction showing how particles arriving at  $z = z_{mirror}$ , which is chosen in the logarithmic layer, are reflected back in the domain so as to respect a zero-mass flux in the wall-normal direction as well as the momentum exchange due to friction in the longitudinal direction.  $\mathbf{U}_p^{in}$  (oriented upward) and  $\mathbf{U}_p^{out}$  (oriented downward) stand for the inward and outward velocities, respectively

208 part of the Langevin models, which is not relevant to the present discussion.  
 209 There are, however, always small differences between the numerical predictions  
 210 of  $\langle \mathbf{U}_f \rangle(t, \mathbf{x})$  and  $\langle \tilde{\mathbf{U}}_p \rangle(t, \mathbf{x})$ . Consequently, Eq. 3 means that the resulting  
 211 mean velocity field obtained from the Lagrangian solver  $\langle \tilde{\mathbf{U}}_p \rangle(t, \mathbf{x})$  is only  
 212 approximately a divergence-free field. A more precise implementation consists  
 213 in writing

$$dU_{p,i} = -\frac{1}{\rho_f} \frac{\partial P^E}{\partial x_i} dt - \frac{1}{\rho_f} \frac{\partial \delta P}{\partial x_i} dt + dM_i, \quad (4)$$

214 where the pressure increments  $\delta P$  are computed to impose that  $\text{div}(\langle \mathbf{U}_p \rangle) = 0$ .  
 215 A classical numerical derivation based on the fractional time-step approach  
 216 yields that  $\delta P$  is the solution of the Poisson equation

$$\frac{\Delta t}{\rho_f} \Delta(\delta P) = \text{div}(\langle \tilde{\mathbf{U}}_p \rangle). \quad (5)$$

217 As such, this correction on particle velocities is equivalent to using a Poisson  
 218 solver twice. As such, better accuracy and consistency is only obtained at the  
 219 cost of doing this operation.

220 In order to test the importance of the correction for particle velocities,  
 221 an approximate method is used where particle velocities in a each cell are  
 222 shifted so that the mean velocity field from the Lagrangian solver is equal to  
 223 the one computed by the Eulerian solver. This is translated by the following  
 224 correction: for each particle labeled  $[k]$ , with  $k = 1, \dots, N_{\mathbf{x}_m}$  where  $N_{\mathbf{x}_m}$  is the  
 225 number of particles located in the cell (here  $m$  refers to cell number and  $\mathbf{x}_m$   
 226 to its center), its instantaneous velocity is modified as

$$U_{p,i}^{[k]}(t) = \tilde{U}_{p,i}^{[k]}(t) - \left( \langle \tilde{U}_{p,i} \rangle(t, \mathbf{x}_m) - \langle U_{f,i} \rangle(t, \mathbf{x}_m) \right) \quad (6)$$

227 to enforce that  $\langle U_{p,i} \rangle(t, \mathbf{x}) = \langle U_{f,i} \rangle(t, \mathbf{x})$  and retrieve a divergence-free mean  
 228 velocity field.

#### 229 2.2.4 Numerical implementation

230 The calculations were performed using *Code\_Saturne*, an open-source CFD  
 231 code developed at Electricité de France Recherche & Développement (EDF  
 232 R&D). Details on the numerical methods implemented in the code can be  
 233 found in Archambeau et al. (2004) for the Eulerian solver and in Peirano et al.  
 234 (2006) for the Lagrangian one.

235 Since the selected numerical cases correspond to steady-state flows, hybrid  
 236 Eulerian/Lagrangian simulations are performed sequentially:

- 237 – first, the Eulerian solver is run and, at convergence, calculations are stopped  
 238 and the mean velocity, pressure, and turbulence fields are frozen. These  
 239 simulations are obtained with the second-order Rotta turbulence model  
 240 (with  $C_R = 4.15$ );
- 241 – second, particles are introduced and tracked within the pre-calculated flow  
 242 fields. The SLM is retained to model fluid particle velocity evolutions (with  
 243  $C_0 = 2.1$ ).

### 244 3 Numerical Assessment

245 In this section, we illustrate the points addressed in Sect. 2 with numerical  
 246 applications. To this end, three cases are studied:

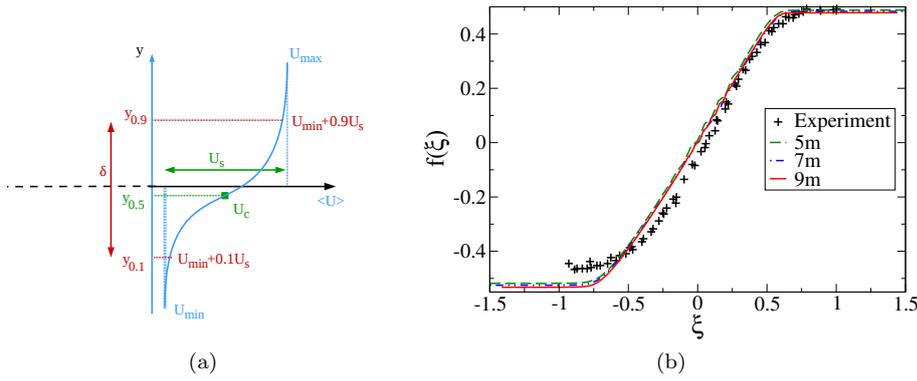
- 247 – a mixing layer (free shear-flow);
- 248 – an infinite channel flow (simple wall-bounded flow);
- 249 – a flow around an obstacle in a boundary layer (complex wall-bounded flow).

250 These three cases allow testing of theoretical and numerical formulations in  
 251 situations where different effects come into play. The mixing layer case is a non-  
 252 homogeneous turbulent flow, with a laminar/turbulent transition at the edges  
 253 of the mixing layer but without flow reversal or wall effects. On the other hand,  
 254 the infinite channel flow is a simple one-dimensional but non-homogeneous  
 255 flow. Finally, the case of the flow around an obstacle located on a wall in a  
 256 atmospheric boundary layer gathers all difficulties: it is a non-homogeneous  
 257 turbulent flow, involving wall effects and complex flow recirculation patterns  
 258 that make it a stringent test case to assess the respect of the well-mixed  
 259 criterion and consistency requirements.

#### 260 3.1 The Mixing Layer Case

##### 261 3.1.1 Case and Simulation Description

262 *Case description* Mixing layers correspond to turbulent flows formed between  
 263 two uniform, nearly parallel streams of different flow speeds  $U_{max}$  and  $U_{min}$ .  
 264 Figure 2a displays the typical sketch of a mixing layer created by the interac-  
 265 tion between two streams with different flow speeds.



**Fig. 2** Sketch and profile of a mixing layer. (a) Sketch of a 2D mixing layer (with the characteristic parameters used and the velocity profile). (b) Profile of the scaled mean longitudinal velocity across the mixing layer: experiments (symbols) and simulations (lines) at various distances from the inlet

266 *Simulation set-up* Numerical simulations of the fluid flow are performed within  
 267 a rectangular domain, whose dimensions are  $10 \text{ m} \times 0.8 \text{ m} \times 0.004 \text{ m}$ , with  
 268 two different inlet velocities. The grid is composed of  $100 \times 100 \times 1$  rectan-  
 269 gular uniform cells. The boundary conditions are as follows: the inlet condi-  
 270 tions on the left-hand side (l.h.s.) of Fig. 2a are divided in two regions,  
 271 each with a uniform velocity profile ( $U = 2 \text{ m s}^{-1}$  for  $y < 0.4 \text{ m}$  and  
 272  $U = 3 \text{ m s}^{-1}$  for  $y > 0.4 \text{ m}$ ); the upper and lower boundaries are symmetry  
 273 (zero-flux) conditions while an outlet condition is applied on the right-hand  
 274 side of Fig. 2a. Thus, the parameters used for dimensionless quantities are  
 275 equal to:  $U_{\min} = 2 \text{ m s}^{-1}$  and  $U_s = 1 \text{ m s}^{-1}$ .

276 Once a stationary regime is reached for the fluid flow, fluid particles are  
 277 then injected until a steady-state regime is reached (i.e. with a statistically-  
 278 constant number of particles. In numerical simulations, each fluid particle rep-  
 279 represents an equal amount of fluid mass and, consequently, the number of par-  
 280 ticles being injected through the two inlet subsections corresponding to the  
 281 two different streams must be so that the inlet mass flow rates are respected.  
 282 Then, given the velocities imposed at the inlet for the two streams ( $2 \text{ m s}^{-1}$   
 283 for  $y < 0.4 \text{ m}$  and  $3 \text{ m s}^{-1}$  for  $y > 0.4 \text{ m}$ ), it was chosen to inject 80 par-  
 284 ticles during each timestep through the low-speed stream inlet (for  $y < 0.4 \text{ m}$ ),  
 285 which means that 120 particles were injected through the high-speed stream  
 286 one (for  $y > 0.4 \text{ m}$ ). When a steady-state was reached, the domain contained  
 287 a number of particles of the order of  $N = 80\,000$ , i.e. about 8 particles per cell.  
 288 In the steady-state regime, Monte Carlo estimates were averaged over time,  
 289 using an ergodic assumption, to reduce statistical noise to low levels: here,  
 290 results have been averaged over 2000 timesteps, meaning that 16000 particles  
 291 per cell were used to calculate statistics.

### 3.1.2 Numerical results

*Self-similarity of the flow* Numerous studies have shown that the flow becomes self-similar after an initial adjustment period and that the flow can be written simply in terms of a scaled velocity (more details can be found in Champagne et al. (1976); Pope (2000)) as follows

$$f(\xi) = \frac{\langle U \rangle - U_c}{U_s}, \quad (7)$$

which depends only on the scaled cross-stream location (self-similar flow)

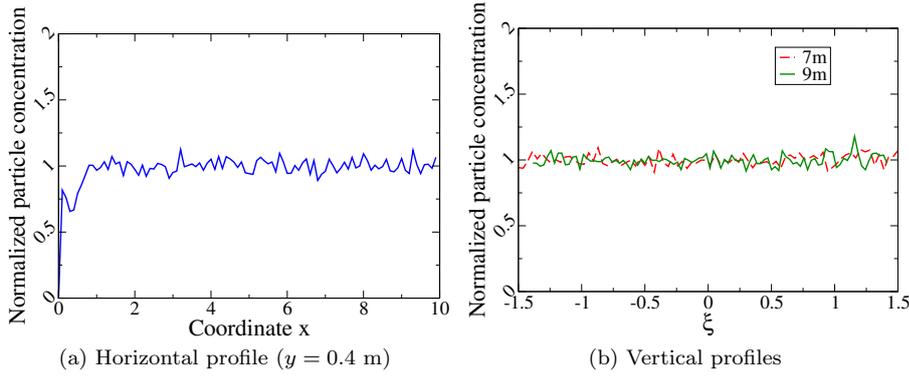
$$\xi = \frac{y - \bar{y}(x)}{\delta(x)}. \quad (8)$$

where  $U_c = \frac{1}{2}(U_{max} + U_{min})$  is the characteristic convection velocity,  $U_s = (U_{max} - U_{min})$  is the characteristic velocity difference,  $\delta(x) = y_{0.9}(x) - y_{0.1}(x)$  is the characteristic width of the flow (defined as the extent of the region where the fluid velocity ranges from  $U_{min} + 0.1U_s$  to  $U_{min} + 0.9U_s$ ) (see Fig. 2a). This self-similarity is well captured by the numerical simulations as appears from the scaled longitudinal mean velocity profiles (see Fig. 2b). Similarly, the Reynolds stresses have been shown to be self-similar when scaled by  $U_s^2$  (not shown here).

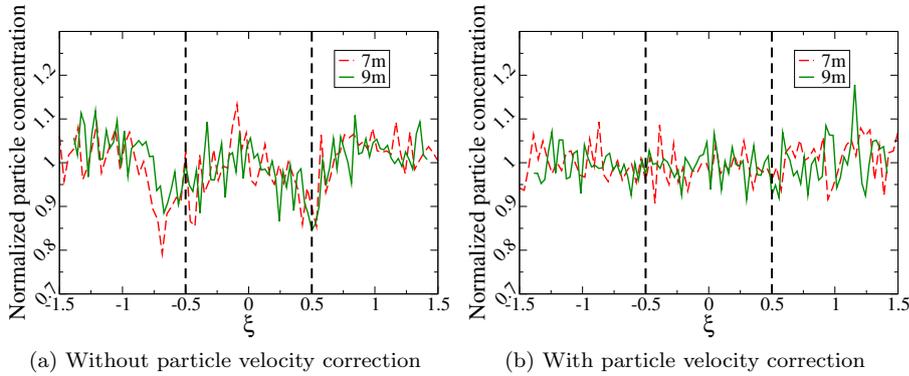
*Well-mixed criterion* Since the objective of the simulation is to assess whether the well-mixed criterion is respected, we consider the normalized particle concentration and check that it remains constant in the simulation domain (particles should not accumulate in nor be removed from regions). The relevant statistical measure is the normalized particle number, or particle concentration, obtained by dividing the actual number of particles in any cell by the mean one.

This normalized particle concentration is displayed in Fig. 3. The horizontal concentration profile taken at mid height ( $y = 0.4$  m), that is at the same height as the splitter plate, is plotted in Fig. 3a. A depletion zone can be seen near the inlet (roughly between the inlet and  $x = 1$  m, whose value depends on the choice of initial velocities and mesh sizes). This depletion region corresponds to the distance needed for the particles to correctly mix in the domain: particles are indeed injected every timestep exactly on the boundary face (and not within the whole boundary cell). This simple injection procedure has been chosen to show that a properly-formulated Lagrangian stochastic model can mix particles and drive the distribution of particle positions to a uniformly-distributed one. Once correctly mixed, the particles remain homogeneously distributed.

*Role of correction on particle velocities* The influence of the particle velocity correction (see Eq. 6) can be estimated by considering the mixing layer case. When calculations are run without this velocity correction, it is seen from



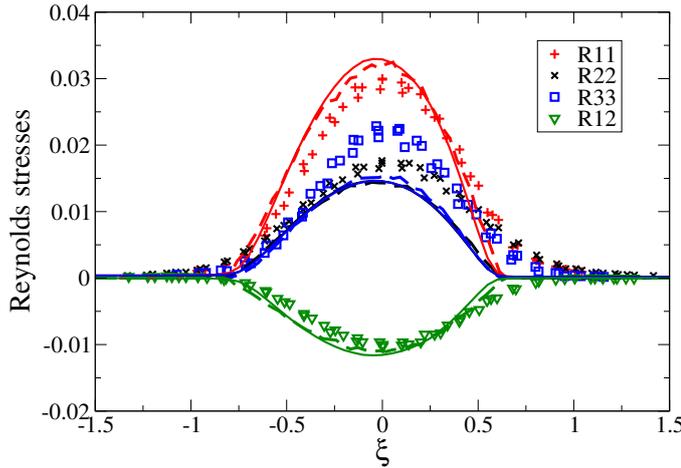
**Fig. 3** Profiles of the particle normalized concentration in the plane mixing layer: (a) sampled longitudinally along the middle of the layer; (b) sampled vertically at various distances from the inlet



**Fig. 4** Profiles of the particle normalized concentration in the mixing layer at various distances from the inlet: comparison between the formulations without and with particle velocity correction (cf. Eq. 6). The dashed lines correspond to the laminar-turbulent transitions

328 Fig. 4a that the normalized-concentration field is only approximately uniform,  
 329 with deviations from unity apparent at the edges of the mixing layer. This is  
 330 related to the fact that the external fluid is entrained to the mixing-layer core,  
 331 where the flow is turbulent, resulting in the external intermittency of the flow.  
 332 However, when this velocity correction is applied, a better result is obtained,  
 333 as revealed by the profiles in Fig. 4b. This confirms that the particle velocity  
 334 correction scheme described in Sect. 2.2.3 is required to obtain more accurate  
 335 results.

336 *Consistency of turbulence models* Scaled Reynolds stresses are extracted from  
 337 the Lagrangian calculation and compared to the ones from the Rotta model  
 338 used in the CFD code. Both predictions of the scaled non-zero second-order  
 339 fluid velocity moments are shown in Fig. 5. It can be seen that the Reynolds  
 340 stresses decrease as expected at the edges of the turbulent region where a tur-



**Fig. 5** Profiles of the scaled Reynolds stresses in the self-similar regime (obtained here at 7 m) for the mixing layer case provided by experimental data (points), the Eulerian solver (continuous lines) and the Lagrangian one (dashed lines) with the consistent hybrid Rotta model/SLM formulation. Both approaches yield nearly-identical predictions for the same second-order velocity moments.

341 bulent/laminar transition is observed. More importantly for our present concern,  
 342 it is clear that numerical results obtained with the Lagrangian model are  
 343 in very good agreement with those obtained with the Eulerian model, indicat-  
 344 ing that consistency is well achieved with the hybrid SLM-Rotta calculation.  
 345 Besides, it can be seen that the numerical results obtained compare fairly well  
 346 to the experimental observations available for the mixing layer case (see also  
 347 Minier and Pozorski (1995) for detailed comparison between numerical and  
 348 experimental results in the mixing layer case).

### 349 3.2 The Infinite Channel Flow

#### 350 3.2.1 Case and Simulation Description

351 *Case description* The second test case corresponds to an infinite half-channel  
 352 flow, which is a simple one-dimensional but non-homogeneous flow. This case  
 353 is representative of wall-bounded flows, i.e. that are affected by the wall-  
 354 boundary conditions.

355 *Simulation set-up* Simulations are performed in a vertical slice of 20 cells,  
 356 with dimensions of  $0.05 \text{ m} \times 0.05 \text{ m} \times 0.05 \text{ m}$ . Since this is basically a one-  
 357 dimensional flow where statistics depend only on the wall-normal coordinate,  
 358 the flow is simply generated by applying a periodicity condition between the  
 359 upstream and downstream faces and by imposing in the longitudinal direction  
 360 a momentum source term that corresponds to the mean pressure gradient (or

361 pressure loss)  $d\langle P_f \rangle / dx = -\rho_f u_*^2 / H$ , where  $\rho_f = 1.18 \text{ kg m}^{-3}$  is the density of  
 362 air,  $H = 1 \text{ m}$  the half-height of the channel, and  $u_* = 0.05 \text{ m s}^{-1}$  the chosen  
 363 value of the friction velocity at the wall.

364 Then,  $N = 200\,000$  particles uniformly distributed over the domain are  
 365 injected. Periodic boundary conditions are applied in the upstream and down-  
 366 stream faces, wall-boundary conditions are applied at the wall while symmetry  
 367 conditions are applied in the other directions. As a result, there is neither in-  
 368 let nor outlet for particles. Particles are then tracked during a time-lapse long  
 369 enough that results truly reflect the governing stochastic model rather than  
 370 the memory of the initial conditions.

### 371 3.2.2 Numerical results

372 *Well-mixed criterion* The purpose of this simulation is to check that a steady  
 373 state is reached, where particle concentration remains uniform across the whole  
 374 channel. As in the mixing layer case, we only consider normalized concentra-  
 375 tions. The average number of particles in a cell is around 10 000, which is  
 376 high-enough for statistics to be obtained directly through Monte Carlo esti-  
 377 mations without using any time-averaging. Incidentally, this allows assessment  
 378 of whether statistics remain stationary in time.

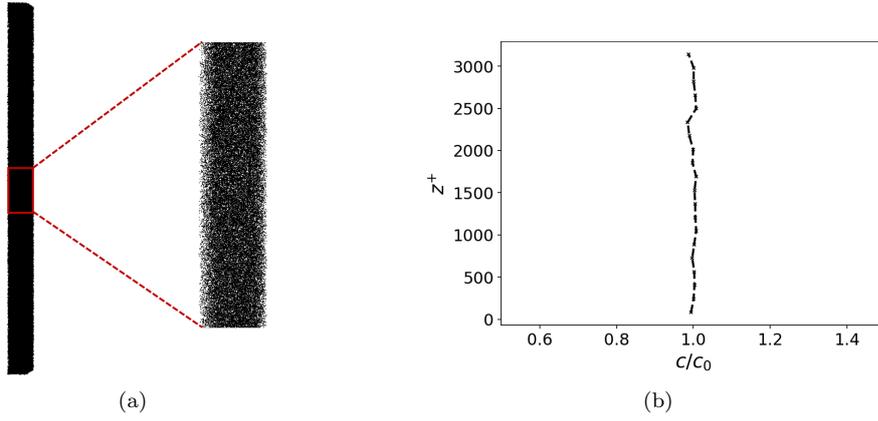
379 Figure 6 shows a scatter plot of particle positions in the domain at the  
 380 end of the calculation, along with the corresponding concentration vertical  
 381 profile derived from it. It can be seen that the concentration is constant over  
 382 the whole height of the channel, indicating that a truly uniform particle dis-  
 383 tribution is obtained. For a more quantitative analysis, the vertical profiles  
 384 of the normalized concentration  $c/c_0$  (where  $c_0$  is the mean concentration in  
 385 the whole domain) derived at different timesteps in the calculation are dis-  
 386 played in Fig. 7a. These profiles show that uniformity across the channel is  
 387 maintained in time. Besides, it can be seen that the normalized concentration  
 388 profiles oscillate with some noise around 1 and it is interesting to analyze the  
 389 nature of these fluctuations. For that purpose, we consider the global spatial  
 390 error defined as

$$\frac{\sigma_c}{c_0} = \frac{1}{c_0} \sqrt{\frac{\sum_{j=1}^{N_{cells}} (c(\mathbf{x}_j) - c_0)^2}{N_{cells}}}, \quad (9)$$

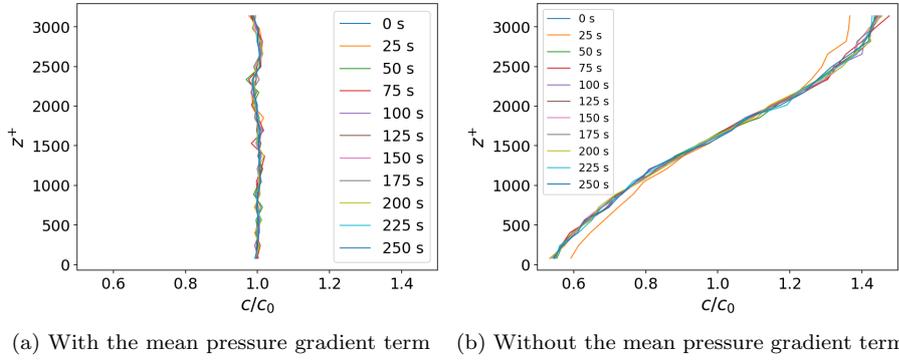
391 where  $N_{cells} = 20$  is the number of cells and  $\mathbf{x}_j$  denotes the position of the  
 392 center of the computational cells. Particle concentration is uniform in the  
 393 domain if and only if the global spatial error  $\sigma_c/c_0$  equals zero. In the present  
 394 case, it is found to be 0.626% at the end of the calculation. However, since we  
 395 are dealing with Monte Carlo estimates, statistical error needs to be accounted  
 396 for. From the Central limit theorem, this error writes

$$\left( \frac{\sigma_c}{c_0} \right)_{Monte\ Carlo} = \sqrt{\frac{N_{cells}}{N}}, \quad (10)$$

397 where  $N$  is the number of particles in the domain. With present values, this  
 398 Monte Carlo error is therefore equal to 1%. Finally, the local error in each



**Fig. 6** Particle repartition at the end of the calculation (a) and the corresponding profile of the particle concentration (b), showing the respect of the well-mixed criterion



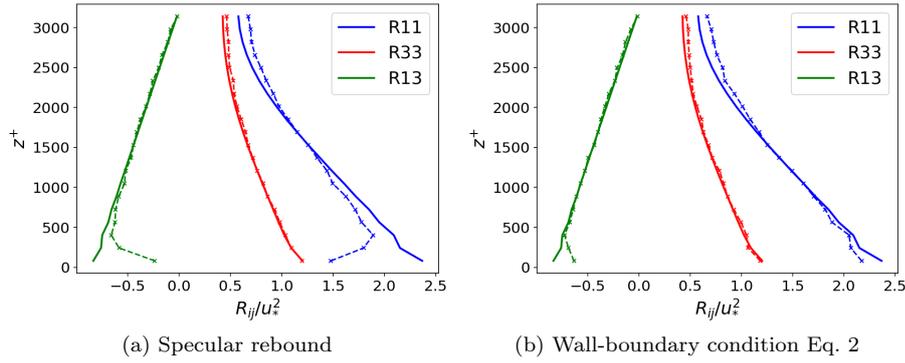
(a) With the mean pressure gradient term (b) Without the mean pressure gradient term

**Fig. 7** Vertical profiles of the normalized particle concentration ( $c/c_0$ ) at different timesteps: (a) with the mean pressure gradient term; (b) without it

399 cell (defined as  $(c - c_0)/c_0$  and evaluated after the solution has reached a  
 400 steady state and  $c$  a constant value) is found to remain within -1.48% and  
 401 0.074%, which confirms that a uniform particle distribution is achieved across  
 402 the height of the channel.

403 *Role of pressure gradient term* As revealed by the normalized concentration  
 404 profiles shown in Fig. 7b, particles tend to accumulate at the top of the domain  
 405 when the mean pressure gradient term is removed from the Langevin  
 406 model (see Sect. 2.1). In the case of the infinite channel flow, it is easy to  
 407 understand why: in the absence of the mean pressure-gradient term, particles  
 408 are driven towards low-energy zones. Indeed, the classical expression of the  
 409 mean-momentum balance equation in the wall-normal direction gives that

$$\frac{1}{\rho_f} \frac{d\langle P_f \rangle}{dz} + \frac{dR_{33}}{dz} = 0, \quad (11)$$

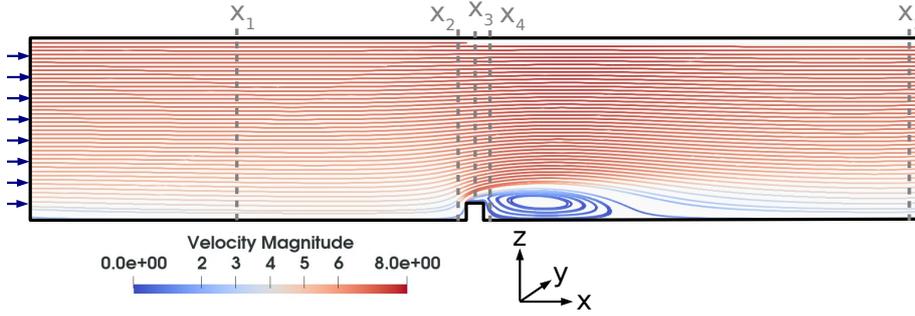


**Fig. 8** Reynolds stress vertical profiles for the case of the infinite plane channel: comparison between two versions of wall-boundary conditions with the consistent hybrid Rotta/SLM formulation. In both versions, consistency is assessed by checking the similarity of the predictions from the Eulerian solver (continuous lines) and the Lagrangian one (dashed crosses)

410 showing that removing the pressure-gradient term is equivalent to a spurious  
 411 particle driving force along the direction of  $dR_{33}/dz$ . In that case, significant  
 412 errors (reaching values up to 30.8%) are introduced, indicating that the general  
 413 formulation without the mean pressure-gradient is deeply flawed.

414 *Consistency of boundary conditions* The profiles of the non-zero Reynolds  
 415 stresses are displayed in Fig. 8. The effect of using consistent wall-boundary  
 416 conditions can clearly be observed: the agreement between the Reynolds-stress  
 417 values extracted from the Eulerian and Lagrangian solvers is much better with  
 418 the current boundary conditions (see Sect. 2.2.2) than when specular rebound  
 419 is used. In particular, the improvement is notable for  $R_{11}$  and  $R_{13}$  with the  
 420 difference between Eulerian and Lagrangian values being reduced by half. It  
 421 can be seen that  $R_{33}$  is not affected, which makes sense since the normal  
 422 velocity component remains unchanged (see Eq. 2). The difference between  
 423 the resulting profiles of the shear stress  $R_{13}$  is noteworthy since this is the key  
 424 element of near-wall turbulent boundary layers (also called constant-stress lay-  
 425 ers) when the viscous sublayer is bridged: applying a specular rebound yields  
 426 a zero-flux condition for the mean longitudinal velocity component and a zero  
 427 shear stress completely at odd with classical laws of wall-boundary layers at  
 428 high Reynolds-number turbulent flows.

429 In practical numerical formulations of wall-boundary conditions, specific  
 430 discretizations are sometimes used. This is the case for the present implemen-  
 431 tation of wall-conditions in the CFD code *Code\_Saturne*, which can explain re-  
 432 maining differences in the numerical outcomes. Further work needs to be done  
 433 to ensure a full correspondence down to the actual numerical formulations.  
 434 Nevertheless, it can be concluded that wall-boundary conditions are necessary  
 435 in Lagrangian stochastic formulations and must be implemented consistently  
 436 with the ones applied in the Eulerian solver when a hybrid formulation is used.



**Fig. 9** Geometry, streamlines and velocity field of a flow around an obstacle within a boundary layer. It reveals the complexity of the flow patterns around the obstacle with a double recirculation on top and downstream. The figure also displays the vertical positions at which profiles are measured

### 3.3 Obstacle within a Boundary Layer

#### 3.3.1 Case and Simulation Description

*Case description* The third test case studied in this work corresponds to a flow around a square obstacle placed on the bottom wall inside a boundary layer. The spanwise dimension of the square obstacle is large enough to be regarded as infinite with respect to other characteristic lengths and the mean flow is therefore a 2D flow. This test case is representative of flows over large obstacles that are usually addressed in atmospheric dispersion studies (as for instance the flow over a building). Yet, as the other cases described earlier in this paper, we are considering a simplified situation. In that sense, these simulations correspond to a ‘verification test case’, meaning that we are checking that the formulation for the model of the fluid flow and for the model of particle dynamics are consistent, and not to a ‘validation case’ (where results are compared to experimental data).

*Simulation set-up* The geometry used to perform such simulations is sketched in Fig. 9: the domain corresponds to a box with sizes equal to  $5 \text{ m} \times 0.1 \text{ m} \times 1 \text{ m}$ . The mesh is simply made up by 798 400 cubic cells. The case considered is a rough boundary layer consisting of a smooth surface with a building (similar to what could be simulated in a wind tunnel with a smooth test section). The flow is initialized with a uniform flow (given also by the same upstream profile). The boundary conditions are thus as follows: the inlet condition reproduces the flow features typical of rough boundary layers (with a roughness height  $z_0$ ), as detailed in Table 3 (note that with the present dimensions, the mean longitudinal velocity component ranges from a near-zero value close to the wall to about  $10 \text{ m s}^{-1}$  at the upper boundary plane); a symmetry condition is applied on the upper boundary while a smooth wall condition is applied to the bottom boundaries.

**Table 3** Inlet dynamical fields for the case of the obstacle within a boundary layer

Field	Value or expression
$\langle U_{f,x} \rangle$ (m s <sup>-1</sup> )	$\frac{u_*}{\kappa} \ln \left( \frac{z + z_0}{z_0} \right)$
$\langle U_{f,y} \rangle$ (m s <sup>-1</sup> )	0
$\langle U_{f,z} \rangle$ (m s <sup>-1</sup> )	0
$u_*$ (m s <sup>-1</sup> )	0.5
$k$ (m <sup>2</sup> s <sup>-2</sup> )	$\frac{u_*}{\sqrt{C_\mu}}, C_\mu = 0.09$
$\epsilon_f$ (m <sup>2</sup> s <sup>-3</sup> )	$\frac{u_*^3}{\kappa(z + z_0)}, \kappa = 0.42, z_0 = 0.0025 \text{ m}$
$\langle U_{f,x}^2 \rangle$ (m <sup>2</sup> s <sup>-2</sup> )	$(2/3) k$
$\langle U_{f,y}^2 \rangle$ (m <sup>2</sup> s <sup>-2</sup> )	$(2/3) k$
$\langle U_{f,z}^2 \rangle$ (m <sup>2</sup> s <sup>-2</sup> )	$(2/3) k$
$\langle U_{f,x}^i U_{f,y}^j \rangle$ (m <sup>2</sup> s <sup>-2</sup> )	0
$\langle U_{f,x}^i U_{f,z}^j \rangle$ (m <sup>2</sup> s <sup>-2</sup> )	$-u_*^2$
$\langle U_{f,y}^i U_{f,z}^j \rangle$ (m <sup>2</sup> s <sup>-2</sup> )	0

464 In order to test different initialization procedures, particle simulations were  
 465 not run starting from an initially void-of-particle domain as for the mixing  
 466 layer case but by initializing a large number of particles ( $N_{ini} = 2\,928\,000$ ) in  
 467 the domain with a uniform position distribution to respect incompressibility. In  
 468 each cell, particle velocities were initialized by sampling in a Gaussian distribu-  
 469 tion determined by the local value of the mean fluid velocity and second-order  
 470 moments (the local value of the Reynolds-stress tensor). Unlike the infinite  
 471 channel flow situation, this is a case with exit and inlet sections but with no  
 472 periodic conditions. Therefore, during each timestep, a number of fluid parti-  
 473 cles ( $N_{inlet} = 352$ ) are injected through the inlet section, according to the  
 474 profile of the inlet mass flow rate. More precisely, for each cell  $k$  corresponding  
 475 to height  $z_k$ :  $N_k = (q_k/Q)N_{inlet}$ , where  $N_k$  is the number of particles in cell  
 476  $k$  and  $Q$  the global fluid flow rate at the inlet. Also,  $q_k = \langle U_f \rangle_k S_k$ , where  
 477  $\langle U_f \rangle_k$  is the mean fluid velocity in cell  $k$  and  $S_k$  is the surface of the boundary  
 478 face related to cell  $k$ . Since the simulation is initialized with a uniform flow,  
 479 we run the simulation until a stationary state is reached. This also ensures  
 480 that particles lose memory of the initial conditions. Results plotted in the  
 481 later figures are thus not influenced by the initial conditions of the simulation.  
 482 Nevertheless, this initialization is useful for avoiding the time-consuming ex-  
 483 plicit simulation of the transient period where particles have to fill the whole  
 484 domain and acts as an accelerator of convergence. When a steady-state is  
 485 reached, the typical number of particles present in the domain is in the order  
 486 of  $N = 3\,000\,000$ , i.e. about 4 particles per cell. Therefore, to extract reli-  
 487 able statistics, a time-averaging procedure is applied as in the mixing layer  
 488 case. To ensure results independent of the number of samples, time averaging  
 489 is performed over 200 000 timesteps (meaning that, on average, statistics are  
 490 estimated with around 800 000 particles in each cell).

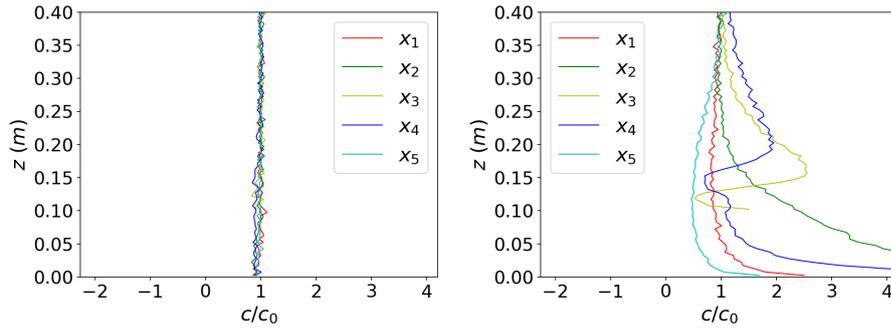
491 Note that for this case, no typical scales can be used in the whole domain,  
 492 as  $u_*$  is not a constant and there is no self-similarity. Therefore, apart from the  
 493 mean concentrations, plots are displayed in terms of dimensional variables.

### 494 3.3.2 Numerical Results

495 *Fluid flow* Fluid phase simulations are run until a statistically steady-state is  
 496 reached. As expected, a strongly non-homogeneous flow is induced by the im-  
 497 pact of the incoming stream on the obstacle, with high levels of kinetic energy  
 498 in the high-shear region appearing downstream of the obstacle. A large recir-  
 499 culation zone is formed downstream of the obstacle but a zoom of the region  
 500 just above the obstacle indicates that another recirculation is created between  
 501 the top wall of the obstacle and the main stream flowing above. This case thus  
 502 represents a very complex flow structure, involving wall effects, recirculating  
 503 and high-shear regions. It is thus a challenging situation for the simulation of  
 504 particle dynamics and, consequently, a severe test to assess the respect of the  
 505 well-mixed criterion.

506 *Well-mixed condition* As for the mixing layer and infinite channel cases, the  
 507 variable of interest is the normalized particle concentration. To assess the  
 508 accuracy of the current approach, the normalized particle concentration is  
 509 sampled along five vertical profiles at various downstream distances from the  
 510 inlet section, as shown in Fig. 9: a first profile is taken upstream of the obstacle  
 511 (sufficiently far from the inlet to have a fully-developed channel flow), three  
 512 profiles just before, above, and just downstream of the obstacle and a last one  
 513 at the end of the domain downstream of the obstacle. The five selected profiles  
 514 of the normalized concentration are shown in Fig. 10a: these profiles confirm  
 515 that a relatively well-mixed condition is obtained as all the different profiles  
 516 remain fairly constant with some fluctuations inherent to particle stochastic  
 517 simulations. The results close to the boundary are not perfect though (particles  
 518 are less present). This may be due to the complex flow structure, which is  
 519 not properly captured with the current log-normal boundary conditions used.  
 520 Improvements of these boundary conditions to better fit this case are left  
 521 out of the present paper but will be investigated in the near future. Given  
 522 the challenging flow structure on the top of the obstacle, the fact that the  
 523 normalized particle concentration remains relatively spatially and temporally  
 524 uniform is a noteworthy result. The global spatial error, defined in Eq. 9, is  
 525 5.06% at the end of the calculation and is therefore satisfactorily low.

526 However, when the mean pressure gradient term is not taken into account in  
 527 the SLM (see Sect. 2.2.3), a completely different picture emerges with marked  
 528 deviations of particle concentration from uniformity, with strong accumulation  
 529 upstream of the obstacle (where fluid streamline curvatures are important) and  
 530 zones of depletion downstream of the obstacle (in the recirculation region).  
 531 When profiles of the normalized concentration are extracted at the same five  
 532 locations, it appears from the plots in Fig. 10b that severe errors are present,  
 533 with some values reaching as high as four times the correct one. In that case,



(a) With the mean pressure gradient term (b) Without the mean pressure gradient term

**Fig. 10** Vertical profiles of the particle normalized concentration at the five sections indicated in Fig. 9 for the case of the flow around an obstacle within a boundary layer. Comparison between the formulations with and without the mean pressure gradient in the SLM. In Fig. 10b, the  $x_2$  and  $x_4$  profiles are not entirely visible because, for these profiles, the ratio  $c/c_0$  reached values up to over 20 (showing a deep violation of the well-mixed criterion). Therefore, for the sake of readability and keeping the same scales for both figures, the  $x$ -scale has been contracted for Fig. 10b

534 the global error is measured as high as 52.8%. This is clearly an unacceptable  
535 level of error, which invalidates such formulations of dispersion models.

536 *Correction of particle positions* The correction on particle velocities introduces  
537 a somewhat asymmetric treatment of particle positions and velocities, since  
538 the evolution equations for  $(\mathbf{X}_p, \mathbf{U}_p)$  can be written as:

$$d\tilde{\mathbf{X}}_{p,i} = \tilde{\mathbf{U}}_{p,i} dt, \quad (12a)$$

$$d\mathbf{U}_{p,i} = d\tilde{\mathbf{U}}_{p,i} - \frac{1}{\rho_f} \frac{\partial \delta P}{\partial x_i} dt, \quad (12b)$$

539 where the same notation  $\tilde{\mathbf{X}}_p$  for particle positions is used to indicate that this  
540 is a first estimation. Eq. 12a shows that particle positions are influenced by  
541 the velocity correction but only in a sequential manner: once particle velocities  
542 are corrected, particle positions are modified at the following timestep. This  
543 loose coupling can be sufficient in some cases, such as the mixing layer and  
544 infinite channel flow cases, but can be limited for more complex flow patterns  
545 with flow reversals and recirculation. This is the situation met with the flow  
546 around the obstacle in the boundary layer. For this reason, tighter coupling is  
547 needed between particle positions and velocities.

548 In stand-alone PDF approaches (see Minier and Pozorski (1999); Bernardin  
549 et al. (2009); Chauvin et al. (2010)), as well as in Smoothed Particle Hydro-  
550 dynamics (SPH) simulations of incompressible flows (Szewc et al. 2012), this  
551 is done by introducing a specific correction on particle positions, so that the

552 complete system can be represented by

$$dX_{p,i} = \tilde{U}_{p,i} dt + \delta X_{p,i} , \quad (13a)$$

$$dU_{p,i} = d\tilde{U}_{p,i} - \frac{1}{\rho_f} \frac{\partial \delta P}{\partial x_i} dt , \quad (13b)$$

553 where in Eq. 13a the correction term  $\delta X_{p,i}$ , accounts for the integrated effect  
 554 (within each timestep) of the one acting on particle velocities in Eq. 13b.  
 555 This particle correction term is derived by stating that a uniform particle  
 556 concentration field should be obtained. Expressing  $\delta X_{p,i}$  as the integrated  
 557 effect of a potential correcting field  $\delta\phi$ , i.e. with  $\delta X_{p,i} = \partial(\delta\phi)/\partial x_i \Delta t$ , leads to  
 558 the formulation of a second Poisson equation whose solution is this correcting  
 559 potential  $\delta\phi$ . Further details on this numerical implementation with corrections  
 560 on particle velocities and positions can be found in Minier and Pozorski (1999).

561 As for particle velocities, a short-cut method was used to assess whether  
 562 such a complete treatment is needed. To that effect, particle positions are sim-  
 563 ply modified by adding a Brownian-like term to the particle position equation,  
 564 so that we have now

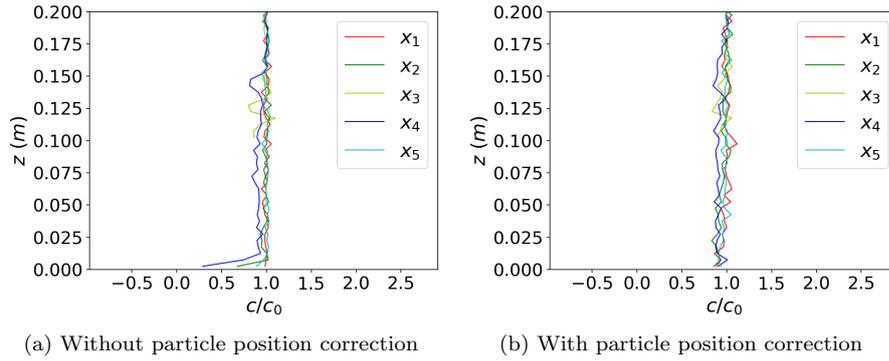
$$dX_{p,i} = \tilde{U}_{p,i} dt + \alpha dW'_i , \quad (14a)$$

$$dU_{p,i} = d\tilde{U}_{p,i} - \frac{1}{\rho_f} \frac{\partial \delta P}{\partial x_i} dt , \quad (14b)$$

565 where  $\alpha$  is a small parameter and  $\mathbf{W}'$  a set of Wiener processes independent of  
 566 the ones used in the Langevin model for particle velocities. This corresponds  
 567 to applying a simple shifting term to particle positions, or a Laplacian term  
 568 in the (Fokker–Planck type of) PDE governing the evolution of the particle  
 569 concentration field.

570 In the case of the flow around the obstacle, this version was used to ob-  
 571 tain the numerical results presented in Sect. 3.3. In the simulations,  $\alpha \approx 0.12$   
 572  $\text{m s}^{-3/2}$ , but  $\alpha$  nevertheless remains an adjustable parameter in the present  
 573 context. The effects of this particle correction scheme can be seen by compar-  
 574 ing results on the particle concentration field with and without that term (cf.  
 575 Fig. 11). Clearly, improved predictions are obtained when the correction term  
 576 is applied. Given the simplified version used in Eq. 14a, this indicates that the  
 577 complete formulation in terms of  $\delta\phi$  as the solution of the corresponding Pois-  
 578 son equation needs to be introduced. This issue will be investigated separately  
 579 in a future study.

580 *Consistency of turbulence models* We now consider the case of the flow around  
 581 an obstacle in a boundary layer, which is more complex since it involves wall  
 582 effects and flow recirculation. Following the analysis in Sect. 3.3, three zones  
 583 (upstream, over, and downstream of the obstacle) are selected where vertical  
 584 profiles are extracted. This is shown in Fig. 12a, c, e for the consistent hybrid  
 585 Rotta-SLM formulation. It can be seen that the profiles computed through the  
 586 Eulerian and Lagrangian approaches are quite similar, especially  $R_{33}$  where  
 587 the identity is almost perfect. There are, however, small differences for  $R_{11}$



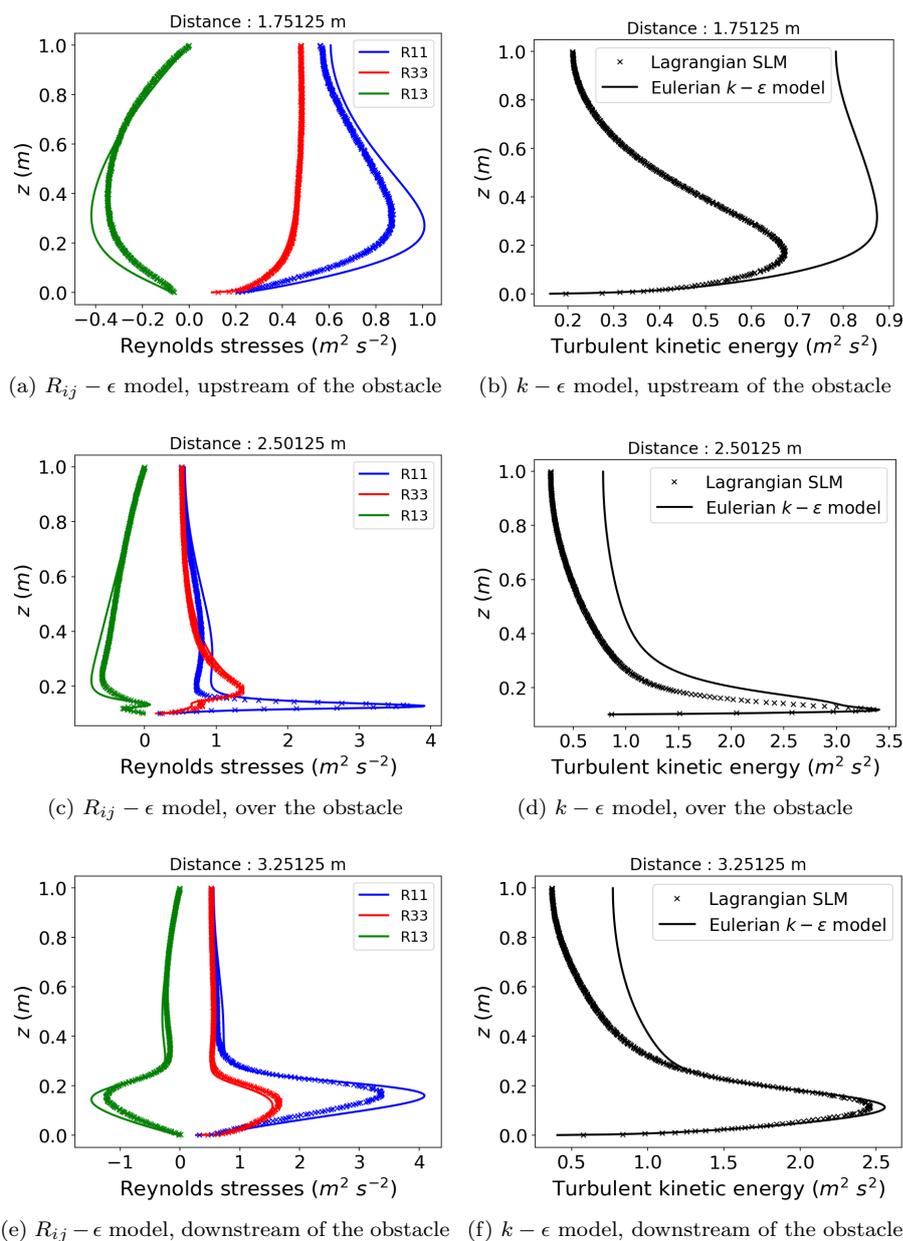
**Fig. 11** Vertical profiles of the particle normalized concentration at the five sections shown in Fig. 9 for the case of the flow around the obstacle within a boundary layer: comparison between the formulations with and without particle position correction, Eq. 14a. The particle velocity correction, Eq. 6, is applied in both formulations

588 values, which is the longitudinal fluid kinetic energy. At that stage, it must  
 589 be recalled that, from a numerical point of view, consistency between Eulerian  
 590 and Lagrangian approaches cannot be perfectly enforced since the triple  
 591 moment has to be modeled in the Eulerian formulation (usually through a  
 592 Daly-Harlow closure) while it is treated without approximation by particle-  
 593 based approaches. Over the obstacle, second-order moments are in a very good  
 594 agreement, which is a noteworthy result given the possible difficulties caused  
 595 by the strong recirculating flow patterns present in the region. In spite of small  
 596 differences that still require further analysis, it can nevertheless be concluded  
 597 that a satisfactory agreement between both Eulerian and Lagrangian results  
 598 are obtained for these duplicate fields, which brings support for the overall  
 599 hybrid formulation.

600 To further illustrate the importance of consistent formulations, another  
 601 simulation was performed using the  $k - \epsilon$  turbulence model for the Eulerian  
 602 calculation. Results are shown in Fig. 12b, d, f, which displays the turbulence  
 603 kinetic energy vertical profiles at the same locations as the ones used with the  
 604  $R_{ij} - \epsilon$  Rotta model for the Eulerian solver (Fig. 12a, c, e). It is obvious that  
 605 significant discrepancies are observed between predictions of the same physical  
 606 quantity, proving that this hybrid formulation is inconsistent and, therefore,  
 607 invalid for reliable predictions.

## 608 4 Conclusions and Perspectives

609 The purpose of the present study is to help the development and use of La-  
 610 grangian stochastic models for atmospheric dispersion applications by clarify-  
 611 ing, through theoretical considerations and a range of numerical situations, the  
 612 issues of the well-mixed condition and consistencies between duplicate fields  
 613 in hybrid Eulerian/Lagrangian simulations.



**Fig. 12** Reynolds stresses and turbulence kinetic energy vertical profiles at various distances from the inlet obtained with the hybrid Rotta model/SLM ((a), (c), (e)) and  $k - \epsilon$ /SLM ((b), (d), (f)) formulations, for the case of the flow around an obstacle within a boundary layer. The predictions correspond to the result of the Eulerian solver (continuous lines) and the Lagrangian one (crosses). With the Rotta model/SLM formulation, consistent duplicate predictions are obtained, whereas the  $k - \epsilon$ /SLM formulation gives inconsistent predictions for the fluid kinetic energy

614 First of all, it has been recalled that the respect of the well-mixed condi-  
615 tion is ensured when the mean pressure-gradient term is correctly introduced  
616 as the mean drift term of Langevin models for the evolution of instantaneous  
617 fluid particle velocities. This has been demonstrated by numerical results ob-  
618 tained in various configurations that cover a range of challenging situations  
619 involving non-homogeneous, recirculating, and wall-bounded turbulent flows.  
620 These examples also confirm that serious discrepancies result when this term  
621 is absent (with zones of particle depletion and/or accumulation).

622 In particle-based models, the incompressibility constraint is translated into  
623 a double one: that the mean velocity derived from particle velocities be of zero  
624 divergence, and that the mean concentration derived from particle positions  
625 remain constant. In practical numerical implementations, this is reflected by  
626 a double correction, first with the introduction of the mean pressure-gradient  
627 term calculated from the zero-divergence condition of the mean flow and, sec-  
628 ond, by a correction step on particle positions. This formulation is valid for  
629 both stand-alone and hybrid Eulerian/Lagrangian numerical codes.

630 In practice, most applications for atmospheric dispersion studies are carried  
631 out with hybrid Eulerian/Lagrangian simulations. This framework has proven  
632 helpful for providing free-of-statistical-noise mean fluid properties (such as  
633 the mean velocity field) from the Eulerian solver to the Lagrangian one. How-  
634 ever, hybrid formulations raise consistency issues for mean fluid properties  
635 predicted both from the Eulerian and Lagrangian models. It is therefore of  
636 paramount importance to realize that the development of improved Eulerian  
637 solvers, through advanced turbulence models, does not necessarily entail that  
638 Lagrangian predictions, based on a given Langevin model, will be improved.  
639 What is central is that both Eulerian and Lagrangian turbulence models be  
640 consistent in such hybrid formulations. In that sense, a second interest of the  
641 present work is to bring out this issue for atmospheric studies and to reveal,  
642 through numerical simulations in a boundary layer, the potentially-damaging  
643 errors induced when inconsistent turbulence models are used. The present  
644 model (coupled with a Rotta model for the Eulerian solver) thus serves as an  
645 illustration of how consistent hybrid formulations can be developed. Future  
646 works are needed to come up with Lagrangian models that are consistent with  
647 LES or Reynolds stress equation models.

648 It is hoped that the present results will be helpful to atmospheric models by  
649 allowing future theoretical and numerical efforts to be safely channeled towards  
650 improved predictions while ensuring that basic conditions and constraints are  
651 satisfied. Indeed, Lagrangian stochastic models have great interest for pas-  
652 sive (as well as reactive) scalar modeling. For example, Bahlali et al. (2018)  
653 have considered point source dispersion and correctly captured the near- and  
654 far-field dispersive behaviors even when using a simple Langevin model. For  
655 future investigations, it will therefore be interesting to extend present consis-  
656 tent hybrid Eulerian/Lagrangian approaches to include scalar modeling based  
657 on more-advanced generalized Langevin model.

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## 666 References

- 667 Alessandrini S, Ferrero E (2009) A hybrid Lagrangian–Eulerian particle model  
668 for reacting pollutant dispersion in non-homogeneous non-isotropic turbu-  
669 lence. *Physica A Stat Mech Appl* 388(8):1375–1387
- 670 Archambeau F, Méchitoua N, Sakiz M (2004) Code Saturne: A Finite Volume  
671 Code for the computation of turbulent incompressible flows - Industrial  
672 applications. *Int J Finite Volumes* 1(1)
- 673 Bahlali ML, Dupont E, Carissimo B (2018) A hybrid CFD RANS/Lagrangian  
674 approach to model atmospheric dispersion of pollutants in complex urban  
675 geometries. *Int J Environ and Pollut* 64(1-3):74–89
- 676 Bernardin F, Bossy M, Chauvin C, Drobinski P, Rousseau A, Salameh T (2009)  
677 Stochastic downscaling method: application to wind refinement. *Stoc Env*  
678 *Res Risk A* 23(6):851–859
- 679 Borgas MS, Flesch TK, Sawford BL (1997) Turbulent dispersion with broken  
680 reflectional symmetry. *J Fluid Mech* 332:141–156
- 681 Cassiani M, Franzese P, Giostra U (2005a) A PDF micromixing model of dis-  
682 persion for atmospheric flow. Part I: development of the model, application  
683 to homogeneous turbulence and to neutral boundary layer. *Atmos Environ*  
684 39(8):1457–1469
- 685 Cassiani M, Franzese P, Giostra U (2005b) A PDF micromixing model of  
686 dispersion for atmospheric flow. Part II: application to convective boundary  
687 layer. *Atmos Environ* 39(8):1471–1479
- 688 Cassiani M, Radicchi A, Albertson JD (2007) Modelling of concentration fluc-  
689 tuations in canopy turbulence. *Boundary-Layer Meteorol* 122(3):655–681
- 690 Champagne FH, Pao YH, Wygnanski IJ (1976) On the two-dimensional mixing  
691 region. *J Fluid Mech* 74(2):209–250
- 692 Chauvin C, Bernardin F, Bossy M, Rousseau A (2010) Wind simulation refine-  
693 ment: some new challenges for particle methods. In: *Progress in Industrial*  
694 *Mathematics at ECMI 2008*, Springer, pp 765–770
- 695 Chibbaro S, Minier JP (2011) A note on the consistency of hybrid Eu-  
696 lerian/Lagrangian approach to multiphase flows. *Int J Multiphas Flow*  
697 37(3):293–297
- 698 De Baas AF, Van Dop H, Nieuwstadt F (1986) An application of the Langevin  
699 equation for inhomogeneous conditions to dispersion in a convective bound-  
700 ary layer. *Q J Roy Meteor Soc* 112(471):165–180
- 701 Dreeben TD, Pope SB (1997) Probability density function and Reynolds-stress  
702 modeling of near-wall turbulent flows. *Phys Fluids* 9(1):154–163

- 703 Franzese P (2003) Lagrangian stochastic modeling of a fluctuating plume in  
704 the convective boundary layer. *Atmos Environ* 37(12):1691–1701
- 705 Lin JC, Gerbig C (2013) How can we satisfy the well-mixed criterion in highly  
706 inhomogeneous flows? A practical approach. *Lagrangian Modeling of the*  
707 *Atmosphere* pp 59–70
- 708 Minier JP (2015) On Lagrangian stochastic methods for turbulent polydisperse  
709 two-phase reactive flows. *Prog Energ Combust* 50:1–62
- 710 Minier JP (2016) Statistical descriptions of polydisperse turbulent two-phase  
711 flows. *Phys Rep* 665:1–122
- 712 Minier JP, Peirano E (2001) The PDF approach to turbulent polydispersed  
713 two-phase flows. *Phys Rep* 352(1):1–214
- 714 Minier JP, Pozorski J (1995) Analysis of a PDF model in a mixing layer case.  
715 In: *Proc. Tenth Symp. Turbulent Shear Flow*, Pennsylvania State University,  
716 pp 26.25–26.30
- 717 Minier JP, Pozorski J (1999) Wall-boundary conditions in probability density  
718 function methods and application to a turbulent channel flow. *Phys Fluids*  
719 11(9):2632–2644
- 720 Minier JP, Chibbaro S, Pope SB (2014) Guidelines for the formulation of  
721 Lagrangian stochastic models for particle simulations of single-phase and  
722 dispersed two-phase turbulent flows. *Phys Fluids* 26(11):113,303
- 723 Monin AS, Yaglom AM (1971) *Statistical fluid dynamics*. MIT Press, Cam-  
724 bridge
- 725 Peirano E, Chibbaro S, Pozorski J, Minier JP (2006) Mean-field/PDF nu-  
726 merical approach for polydispersed turbulent two-phase flows. *Prog Energ*  
727 *Combust* 32(3):315–371
- 728 Pope SB (1985) PDF methods for turbulent reactive flows. *Prog Energ Com-*  
729 *combust* 11(2):119–192
- 730 Pope SB (1987) Consistency conditions for random-walk models of turbulent  
731 dispersion. *Phys Fluids* 30(8):2374–2379
- 732 Pope SB (1991) Computations of turbulent combustion: progress and chal-  
733 lenges. In: *Symposium (International) on Combustion*, Elsevier, vol 23, pp  
734 591–612
- 735 Pope SB (1994a) Lagrangian PDF methods for turbulent flows. *Annu Rev*  
736 *Fluid Mech* 26(1):23–63
- 737 Pope SB (1994b) On the relationship between stochastic Lagrangian models  
738 of turbulence and second-moment closures. *Phys Fluids* 6(2):973–985
- 739 Pope SB (2000) *Turbulent flows*. Cambridge Univ. Press
- 740 Sawford B (1986) Generalized random forcing in random-walk turbulent dis-  
741 persion models. *Phys Fluids* 29(11):3582–3585
- 742 Sawford BL (1985) Lagrangian statistical simulation of concentration mean  
743 and fluctuation fields. *J Clim Appl Meteorol* 24(11):1152–1166
- 744 Sawford BL, Guest FM (1988) Uniqueness and universality of Lagrangian  
745 stochastic models of turbulent dispersion. In: *8th Symposium on Turbulence*  
746 *and Diffusion*, vol 1, pp 96–99
- 747 Stohl A, Forster C, Frank A, Seibert P, Wotawa G (2005) The Lagrangian  
748 particle dispersion model FLEXPART version 6.2. *Atmos Chem Phys*

- 749 5(9):2461–2474
- 750 Szewc K, Pozorski J, Minier JP (2012) Analysis of the incompressibility con-  
751 straint in the smoothed particle hydrodynamics method. *Int J Numer Meth*  
752 *Eng* 92(4):343–369
- 753 Thomson DJ (1987) Criteria for the selection of stochastic models of particle  
754 trajectories in turbulent flows. *J Fluid Mech* 180:529–556
- 755 Tinarelli G, Mortarini L, Castelli ST, Carlino G, Moussafir J, Olry C, Armand  
756 P, Anfossi D (2013) Review and validation of MicroSpray, a Lagrangian par-  
757 ticle model of turbulent dispersion. *Lagrangian Modeling of the Atmosphere*  
758 pp 311–328
- 759 Van Dop H, Nieuwstadt FTM, Hunt JCR (1985) Random walk models for  
760 particle displacements in inhomogeneous unsteady turbulent flows. *Phys*  
761 *Fluids* 28(6):1639–1653
- 762 Waławczyk M, Pozorski J, Minier JP (2004) Probability density function  
763 computation of turbulent flows with a new near-wall model. *Phys Fluids*  
764 16(5):1410–1422
- 765 Wilson JD, Sawford BL (1996) Review of Lagrangian stochastic models for  
766 trajectories in the turbulent atmosphere. Springer
- 767 Wilson JD, Thurtell GW, Kidd GE (1981) Numerical simulation of particle  
768 trajectories in inhomogeneous turbulence, III: Comparison of predictions  
769 with experimental data for the atmospheric surface layer. *Boundary-Layer*  
770 *Meteorol* 21(4):443–463