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# Atmospheric dispersion using a Lagrangian stochastic approach: application to an idealized urban area under neutral and stable meteorological conditions

Meïssam L. Bahlali<sup>a,b,\*</sup>, Eric Dupont<sup>b</sup>, Bertrand Carissimo<sup>b</sup>

<sup>a</sup>Department of Civil and Environmental Engineering, Imperial College London, London, UK

<sup>b</sup>CEREA, Joint laboratory Ecole des Ponts ParisTech/EDF R&D, 6 quai Watier, 78401 Chatou Cedex,  
France

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## Abstract

We present an adaptation of the Lagrangian stochastic dispersion model of the computational fluid dynamics (CFD) open source code *Code\_Saturne* to simulate atmospheric dispersion of pollutants in complex urban geometries or around industrial plants. The wind is modeled within the same code with an Eulerian RANS (Reynolds-averaged Navier-Stokes equations) approach and thus involves the solution for the ensemble-mean velocity field and turbulent moments, using eddy viscosity or Reynolds stress turbulence models adapted to the atmosphere and complex geometries. The Lagrangian stochastic model used for the dispersion of the particles within this flow field is the simplified Langevin model, which pertains to the approaches referred to as PDF (Probability Density Function) methods. This formulation of model has not been widely used in atmospheric applications, despite interesting theoretical and computational benefits. Therefore, its usage must be validated on different atmospheric cases. In this paper, we present the validation of the model with a field experiment, considering atmospheric stratification and buildings: the MUST (Mock Urban Setting Test) campaign, conducted in Utah's desert, USA.

*Keywords:* Atmospheric dispersion, Lagrangian models, Eulerian models, Wind flow modeling, MUST experiment

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## 1. Introduction

An atmospheric dispersion model is a tool that can be used to simulate the atmospheric phenomena involved in the turbulent pollutant dispersion process. The differences between the many existing models to date are mainly in terms of the number of atmospheric processes considered, their degree of complexity, their field of application and, in particular, the methods used to solve the equations governing them. We can distinguish mainly three types of models:

- Gaussian models, based on the analytical resolution of the so-called advection-diffusion equation (on a scalar corresponding to the concentration of pollutant) coupled with semi-empirical parameterizations of the main physical phenomena;

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\*Corresponding author: [meissambahlali@gmail.com](mailto:meissambahlali@gmail.com)

This research was done while M. L. Bahlali was a Ph.D. student at CEREA, in 2015-2018.

- Eulerian models, based on the resolution of the discretized advection-diffusion equation in time and space on a mesh;
- Lagrangian models, based on the computation of particle trajectories.

Eulerian models, when used through Computational Fluid Dynamics (CFD) methods, rely on the resolution of the advection-diffusion equation of a scalar on a mesh. This equation implies the knowledge of the velocity and turbulent fields. Therefore, the first step is the resolution of the Eulerian Navier-Stokes momentum equation, in order to compute the flow field over which the dispersion will be calculated. Generally, the resolution of the Navier-Stokes momentum and scalar transport equations are carried out within the same model. This therefore supposes to have a model that provides a solution for the dynamical fields of high enough quality, since it strongly influences the solution obtained for the concentration field calculated through the advection-diffusion equation. In particular, this highlights the crucial importance of a correct modeling of flow turbulence. This topic has been addressed in various papers as atmospheric simulations using CFD have been increasingly used in the past few decades (Franke et al., 2004; Blocken, 2014), especially at local scale (with, for instance, studies of wind flow patterns at pedestrian level around buildings, see Yoshie et al. (2007); Mochida et al. (2008); Tominaga et al. (2008); Blocken and Stathopoulos (2013)).

On the other hand, Lagrangian models consist of calculating and following the trajectories of particles in a turbulent flow. Thus, the frame of reference is not fixed but follows the cloud described by a large number of particles emitted into the atmosphere. For each of these particles, a stochastic differential equation of a Langevin type is written on their velocity. By integrating over time, we are thus able to get the position of each and then deduce the concentration field over the computational domain. The main strength of Lagrangian models is that they treat convection without any approximation. In particular, they can treat without approximation local source terms when they are provided as known expressions of the variables associated with the particles, such as chemical source terms (Minier, 2015). Also, Lagrangian models are grid-free, which makes them accurate to capture the different turbulent structures in a statistical sense and avoid numerical diffusion problems that can be encountered within Eulerian models – especially near the source. However, one must keep in mind that they usually still depend on a grid in two ways:

- the stochastic differential equation that governs the velocity evolution of the particles usually involves fluid mean quantities that are in practice provided by a grid-based meteorological pre-processor or a CFD calculation;
- the concept of ‘concentration’ is by definition mesh-based.

Both CFD Eulerian and Lagrangian models are well-suited for atmospheric dispersion studies in urban neighborhoods or around industrial plants, in the sense that they are capable of capturing the complex interactions between the air flow and the buildings for different meteorological conditions. However, these two types of models have often been

74 compared ignoring the level of turbulence closure used for each. Loosely speaking, a com-  
75 mon belief is that ‘Eulerian models do not work well near the source’. In reality, a more  
76 correct affirmation would be: ‘Eulerian models that are based on a gradient-diffusion hy-  
77 pothesis do not work well near the source’, since this region corresponds to the short-time  
78 limit where the fully diffusive regime has not been reached yet (Taylor, 1921). In fact, in the  
79 atmospheric dispersion field, Lagrangian models are commonly referred to models simulat-  
80 ing the particle **velocities** as stochastic diffusion processes, which by construction makes  
81 them second-order. On the other hand, a Lagrangian model simulating the **positions** as  
82 stochastic diffusion processes is equivalent to an Eulerian model using a gradient-diffusion  
83 hypothesis. More details can be found on that subject in Minier (2016). To sum up, the  
84 Eulerian/Lagrangian comparisons should not be about the approaches in themselves but  
85 rather about the level of closure that is considered. Throughout this paper, we will be  
86 coming back on this point of significant importance when it comes to rigorously comparing  
87 the accuracy of the results given by both approaches.

88 In the past few years, the constantly increasing computing power has enabled (and  
89 above all made easier) the use of Lagrangian stochastic methods for atmospheric pur-  
90 poses – see for example Franzese (2003), Stohl et al. (2005), Cassiani et al. (2005a,b),  
91 Bernardin et al. (2009), Alessandrini and Ferrero (2009), Tinarelli et al. (2013), etc. For  
92 our work, a simulation tool using a Lagrangian PDF (Probability Density Function) to  
93 carry out pollutant dispersion studies has been developed in the three-dimensional CFD  
94 code *Code\_Saturne* (<http://code-saturne.org/>, see Archambeau et al. (2004) for more  
95 details). It has been validated on simple academic cases and **shown** to satisfactorily re-  
96 spect the well-mixed condition (see Bahlali et al. (2018a,b)). This paper is concerned with  
97 validating the model in real conditions by studying continuous point source dispersion of  
98 a non-reactive pollutant in an idealized urban area, as such a case is typical **of industrial**  
99 **emissions or an** accidental release.

100 The present work will focus on the Mock Urban Setting Test (MUST) campaign, which  
101 has been widely studied in the literature. For previous numerical simulations of the ex-  
102 periment, the reader may for example refer to Hanna et al. (2004), Camelli et al. (2005),  
103 Donnelly et al. (2009), Antonioni et al. (2012), Kumar et al. (2015). Comparisons between  
104 different modeling systems have also been studied: Santiago et al. (2010) and Dejoan  
105 et al. (2010) compared large-eddy simulations (LES) to Reynolds-averaged Navier-Stokes  
106 (RANS) computations, and Castelli et al. (2017) performed comparisons between different  
107 atmospheric Eulerian and Lagrangian modeling approaches. Experimental comparisons  
108 have been conducted as well: Leitl et al. (2007) worked on the Hamburg wind tunnel  
109 experiment, **and** Yee et al. (2006) compared experimental wind-tunnel and water-channel  
110 simulations.

111 In the CFD code *Code\_Saturne*, previous numerical simulations of the MUST campaign  
112 have also already been performed by Milliez and Carissimo (2007, 2008) and used an  
113 Eulerian  $k - \epsilon$  model of turbulent dispersion. The present work aims at studying the same  
114 cases using the Lagrangian stochastic model. The objective is twofold:

- 115 • first, we would like to assess the accuracy of the results provided by the Lagrangian  
116 model for this specific industrial application;
- 117 • second, we would like, in the same CFD simulations, to compare the Lagrangian  
118 results to the ones obtained with several Eulerian turbulence models, and above all  
119 explain the differences to provide a better understanding of the different modeling  
120 options.

121 A specificity of this work is that the wind is modeled *within the same code* as the  
122 dispersion, with an Eulerian RANS approach. It thus involves the solution for the ensemble-  
123 mean velocity field and turbulent moments, using  $k-\epsilon$  or second-moment  $R_{ij}-\epsilon$  turbulence  
124 closures adapted to the atmosphere and complex geometries. In the aforementioned nota-  
125 tions,  $k$  is the turbulent kinetic energy (TKE),  $\epsilon$  the turbulent dissipation rate and  $R_{ij}$  the  
126 Reynolds stress tensor. Note that Milliez and Carissimo (2007, 2008) only simulated the  
127 wind dynamical mean fields using a  $k-\epsilon$  model. Therefore, in addition to the Lagrangian  
128 results, this paper will also expose new results on the Eulerian approach through the use  
129 of the second-order  $R_{ij}-\epsilon$  model for the wind mean quantities.

130 This paper will be organized as follows. First, both the Eulerian and Lagrangian model  
131 equations used in this work will be introduced. Second, the experiment characteristics will  
132 be exposed and the two cases chosen for this study will be described. Finally, results for  
133 both these cases will be shown and the different modeling approaches will be discussed.

## 134 2. Model equations

135 The methodology for atmospheric dispersion calculations in *Code\_Saturne* consists of  
136 two simulations:

- 137 • the first simulation solves the mean Navier-Stokes equations for the flow field;
- 138 • the second simulation restarts from the previous frozen flow field (velocity, turbulence  
139 and temperature) and computes the dispersion.

140 In the following subsections, the different modeling options in Eulerian and Lagrangian  
141 approaches are presented.

### 142 2.1. The Eulerian approach

143 Eulerian models, as explained in the introduction, are based on the resolution of the  
144 mean advection-diffusion equation of a given Reynolds-averaged scalar  $\langle c \rangle$  through its  
145 discretization in time and space on a mesh. This equation is written as:

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

146 where  $U_{f,j}$  is the fluid velocity along the  $j$  axis,  $D$  the molecular diffusivity,  $S$  and  $R$   
 147 respectively the source and reactive terms. Also, the notation  $\langle \rangle$  stands for Reynolds  
 148 average and  $'$  its deviation part.

149 This equation involves the unknown term  $\langle U'_{f,j}c' \rangle$ . For practical applications, two main  
 150 families of closures are considered:

- 151 • eddy diffusivity models, which directly provide a local expression for  $\langle U'_{f,j}c' \rangle$ ;
- 152 • second-order models, which consist of a complete transport of the turbulent scalar  
 153 fluxes  $\langle U'_{f,j}c' \rangle$ .

154 Eddy diffusivity models are widely used in the atmospheric dispersion literature, usually  
 155 through the following simple gradient-diffusion hypothesis:

$$\langle U'_{f,j}c' \rangle = -D_t \frac{\partial \langle c \rangle}{\partial x_j}, \quad (2)$$

156 where  $D_t = \nu_t / Sc_t$ ,  $Sc_t$  being the turbulent Schmidt number, usually ranging  
 157 and 1 for air.

158 In this expression,  $\nu_t = C_\mu k^2 / \epsilon$  is the fluid turbulent viscosity;  $k = (1/2) R_{ii}$  where by  
 159 definition  $R_{ij} = \langle U'_{f,i}U'_{f,j} \rangle$ . In  $k - \epsilon$  models,  $R_{ij}$  is constructed as follows:

$$R_{ij} = (2/3) k - 2 \nu_t S_{ij} \quad (3)$$

160 where  $S_{ij} = (\partial U'_{f,i} / \partial x_j + \partial U'_{f,j} / \partial x_i) / 2$ , so that  $R_{ij}$  is symmetric and  $\text{Tr}(R_{ij}) = 2k$ .

161 An important point to recall here is that if a turbulent-viscosity model is used for the  
 162 resolution of the mean dynamical fields, then obviously, closure of  $\langle U'_{f,j}c' \rangle$  will be performed  
 163 through a 'turbulent-diffusivity' model. On the other hand, one can use a second-order  
 164  $R_{ij} - \epsilon$  model to compute the mean dynamical fields and still use a turbulent-diffusivity  
 165 model for the turbulent scalar fluxes closure (*i.e.*, here, the model of Eq. (2)). The present  
 166 work will provide new elements on that topic, by comparing, using either a  $k - \epsilon$  or a  
 167  $R_{ij} - \epsilon$  model to compute the mean dynamical fields, the results obtained through a tur-  
 168 bulent-diffusivity model for the scalar dispersion. As for second-order scalar fluctuations  
 169 models for meteorological applications, they are in fact still an open and difficult research  
 170 problem, and the subject of further investigations.

## 171 2.2. The Lagrangian approach

172 Let  $\mathbf{X}_p$  be the position of a particle included in the air flow and  $\mathbf{U}_p$  its velocity. Both  
 173 variables are driven by the following system:

$$dX_{p,i} = U_{p,i}(t)dt, \quad (4a)$$

$$dU_{p,i} = -\frac{1}{\rho} \frac{\partial \langle P \rangle}{\partial x_i} dt + (\langle U_{p,i} \rangle - \langle U_{f,i} \rangle) \frac{\partial \langle U_{f,i} \rangle}{\partial x_i} dt - \frac{U_{p,i} - \langle U_{f,i} \rangle}{T_L} dt + \sqrt{C_0 \epsilon} dW_j, \quad (4b)$$

174 where  $dW_j$  are independent Wiener processes. Briefly speaking, a Wiener process is a Gaussian  
 175 process with independent increments of zero mean and with a variance equal to  $dt$   
 176 (more details can be found in Gardiner (1985); Öttinger (1996)). Also,  $T_L = \frac{1}{\frac{1}{2} + \frac{3}{4}C_0} \frac{k}{\epsilon}$  is  
 177 the Lagrangian integral timescale and  $C_0$  is a constant given by Kolmogorov's theory.

178 In Eq. (4b), the sum of the first, second and third terms on the right-hand-side is  
 179 known as the drift term. More precisely, the drift term is the sum of a mean component  
 180 (the mean pressure gradient  $-\frac{1}{\rho} \frac{\partial \langle P \rangle}{\partial x_i} dt$  and the term accounting for the crossing-trajectory  
 181 effect  $\langle U_{p,i} \rangle - \langle U_{f,i} \rangle \frac{\partial \langle U_{f,i} \rangle}{\partial x_i} dt$ , more detailed in the following paragraph) and a fluctuating  
 182 component (the return-to-equilibrium term  $-\frac{U_{p,i} - \langle U_{f,i} \rangle}{T_L} dt$ ). On the other hand, the fourth  
 183 term on the right-hand-side of Eq. (4b) is known as the diffusion term and is defined  
 184 following Kolmogorov's similarity theory.

185 The stochastic differential equation governing the evolution of  $\mathbf{U}_p$  is a model inspired by  
 186 the two-phase flow formulation of Minier and Peirano (2001) and the Simplified Langevin  
 187 Model (SLM) of Pope (2000) – it actually stands between the two of them, the difference  
 188 lying in the  $(\langle U_{p,i} \rangle - \langle U_{f,i} \rangle) \frac{\partial \langle U_{f,i} \rangle}{\partial x_i} dt$  term. The formulation with this term makes sense  
 189 since even though we are dealing with fluid particles (putting us in the single-phase flow  
 190 situation), particles dispersing from a point source can be seen as a subset of the whole  
 191 simulated flow. Therefore, in each cell of the computational domain, their mean velocity  
 192 has no reason to be equal to the fluid velocity, hence the non-null production term on the  
 193 second term of the right-hand-side of Eq. (4b). In fact, for a better understanding, let us  
 194 assume that the whole flow is represented by particles uniformly distributed in the domain  
 195 and affect a scalar  $\alpha$  to each of them:

$$196 \quad \begin{cases} \alpha = 1 & \text{if the particle comes from the source;} \\ \alpha = 0 & \text{if it does not come from the source.} \end{cases}$$

197 Therefore, the condition that the mean particle velocity field needs to observe is:  
 198  $\mathbf{div}(\alpha \langle \mathbf{U}_p \rangle) = \mathbf{0}$ , which is a completely different condition than the one the fluid velocity  
 199 field has to meet, *i.e.*,  $\mathbf{div}(\langle \mathbf{U}_f \rangle) = \mathbf{0}$ .

200 Loosely speaking, this formulation stands in a philosophical line that is close to the  
 201 LRR-IP (Launder, Reece, Rodi - Isotropization of Production) model of Pope (2000),  
 202 except that the production term here is related to the mean particle velocity instead of the  
 203 instantaneous one. This production term actually makes significant physical sense, since  
 204 it adds more anisotropy to the dispersion of the particles. Furthermore, if one studies the  
 205 limiting case of particles modeling the whole flow (*i.e.*, the 'fluid limit'), then it yields  
 206  $\langle U_{p,i} \rangle = \langle U_{f,i} \rangle$  and the SLM is retrieved. More precisely, Bahlali et al. (2018b) have shown  
 207 that the SLM fully respects the well-mixed criterion (as defined in Thomson (1987)) and  
 208 that it is completely consistent with a second-order  $R_{ij} - \epsilon$  (Rotta) turbulence model for the  
 209 fluid phase. Both these conditions are in fact essential for any Lagrangian stochastic model  
 210 of a Langevin type to be regarded as acceptable (see Minier et al. (2014)). In conclusion,  
 211 the model defined in Eq. (4), since it relaxes to the SLM for the fluid limit, is well-mixed

212 and able to reproduce transport equations for the first two moments of the velocity field: it  
213 can thus reasonably be used to simulate point source dispersion in non-homogeneous flows  
214 such as the one studied in this work. However, one must keep in mind that this model  
215 has been developed for neutral conditions. It is possible to use it also for buoyancy-driven  
216 flows, as we did in the present work, but some improvements can be made for these cases  
217 and are the subject of further investigations (cf. conclusion).

218 It should be noted that this Lagrangian model alone does not take into account molecu-  
219 lar diffusion. Indeed, if a scalar  $c$  is added to the state vector associated with each particle,  
220 then:  $dc/dt = 0$  (conservative particles are studied, with a constant concentration along  
221 their trajectories). In order to represent the molecular diffusion phenomenon, a so-called  
222 ‘micro-mixing model’ can be used (see, for example, Villermaux and Devillon (1972); Pope  
223 (2000); Sawford (2004); Luhar and Sawford (2005); Amicarelli et al. (2012); Cassiani et al.  
224 (2015)). This type of model is often used in the case of reactive pollutants, since in this  
225 context molecular diffusion plays an important role. In the case of high Reynolds numbers,  
226 molecular diffusion does not affect the concentration mean (Pope, 1998), and is therefore  
227 generally neglected compared to turbulent diffusion.

### 228 3. The Mock Urban Setting Test experiment

#### 229 3.1. Description of the site

230 The experimental program this paper focuses on is the Mock Urban Setting Test cam-  
231 paign, conducted in Utah’s desert, USA, by the US Defense Threat Reduction Agency  
232 (DTRA). It consists of the release of a pollutant in an idealized urban environment rep-  
233 resented by several rows of containers. The details of the experiment as well as the results  
234 are described in Biltoft (2001) and Yee and Biltoft (2004).

235 It is worth noting that pollutant dispersion simulations in urban geometries using CFD  
236 have been widely studied in the past few years, for instance within street canyons (Tom-  
237 inaga and Stathopoulos, 2011; Salim et al., 2011) or around high-rise buildings (Yoshie  
238 et al., 2011). In this work, the objective is to reproduce some of the simulations of the  
239 MUST campaign that have already been performed in the past by Milliez and Carissimo  
240 (2007, 2008) in *Mercurie* (former name of the atmospheric module of *Code\_Saturne*), but  
241 completing them with new results using the Lagrangian stochastic model previously in-  
242 troduced and the second-order  $R_{ij} - \epsilon$  model for the fluid phase computation. Milliez  
243 and Carissimo (2007) described in detail the characteristics of the campaign, which are  
244 summarized below:

- 245 • 63 emissions of a neutral gas (propylene  $C_3H_6$ ), among which 58 are continuous and  
246 5 are puff releases;
- 247 • flat terrain with some bushes from 50 cm to 1 m high;
- 248 • presence of obstacles through a regular alignment of containers of dimensions 12.2 m  
249 (length)  $\times$  2.42 m (width)  $\times$  2.54 m (height);



Figure 1: Some views of the MUST experiment (after Milliez (2006)).

- 250 • different wind conditions through varying angles of incidence, wind velocities, turbu-  
251 lence, temperature, stability conditions;
- 252 • different release heights: 0.15 m, 1.3 m, 1.8 m, 2.6 m and 5.2 m.

253 Figure 1 shows two photos of the MUST experiment. The regular alignment of the  
254 containers is supposed to represent an idealized city and the objective of the experiment  
255 is to observe the point source dispersion of the propylene continuously released in this  
256 environment. We are interested in checking how the Lagrangian model behaves in the  
257 presence of obstacles in a real situation. Indeed, when assessing the respect of the well-  
258 mixed criterion for the SLM, Bahlali et al. (2018b) studied the case of a non-homogeneous  
259 turbulent flow around an obstacle within a boundary layer and observed notable differences  
260 in the behavior of the particles depending on the turbulence model that was used to  
261 compute the fluid phase.

262 The experimental devices used in the campaign are illustrated in Figure 2. Wind and  
263 temperature measurements were carried out using sonic anemometers (30-m mast S just  
264 upstream of the canopy, 32-m central tower T and 8-m masts A, B, C and D inside the  
265 canopy). As for pollutant concentrations, they were measured by photoionization detectors  
266 (PIDs), positioned on four horizontal lines (*line 1, 2, 3, 4*' in Figure 2). These four lines  
267 were located at height 1.6 m. PIDs were also placed at 6 levels on the masts A, B, C, D  
268 and at 8 levels on the tower T.

269 Finally, it should be noted that the tracer releases occurred at dusk or dawn, thus under  
270 meteorological conditions ranging from stable to neutral. The duration of each release was  
271 15 min and for the analysis of the results, periods of 200 s were extracted by Yee and Biltoft  
272 (2004). These periods were indeed quasi-steady in terms of wind speed and direction and  
273 also remained greater than the plume travel time.

### 274 3.2. Description of the cases studied

275 As previously mentioned, the MUST experiment consisted of 63 tracer releases and in  
276 the work of Milliez and Carissimo (2007, 2008), twenty cases were simulated. In the present

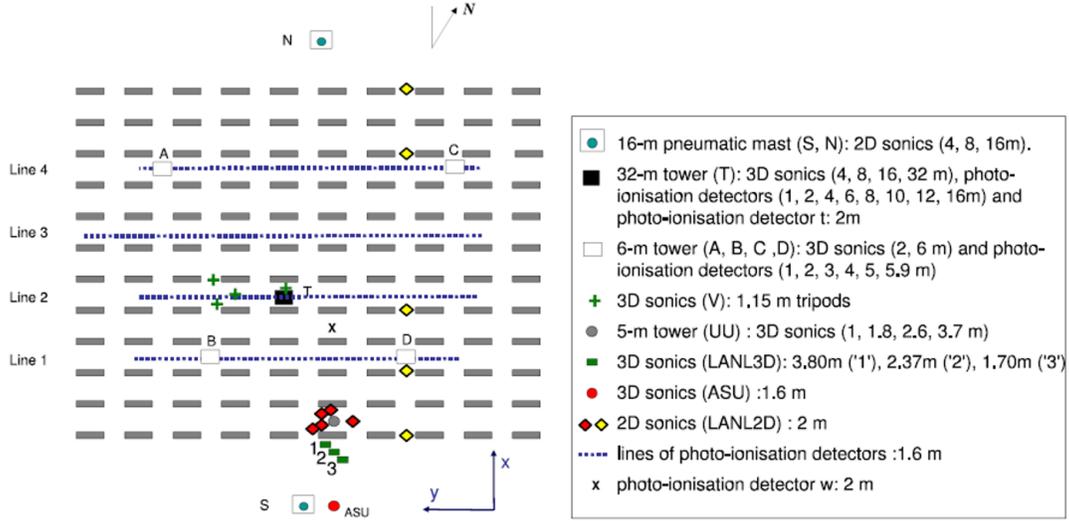


Figure 2: Schematic diagram of the MUST experiment and location of the experimental devices (after Milliez and Carissimo (2008)).

Case	$\alpha_4$ (deg)	$S_4$ (m.s <sup>-1</sup> )	$k_4$ (m <sup>2</sup> .s <sup>-2</sup> )	$L$ (m)	$Q$ (L.min <sup>-1</sup> )	Source location	$z_s$ (m)
2681829	-41	7.93	4.263	28000	225	29	1.8
2692157	43	2.98	0.510	130	225	36	2.6

Table 1: Characteristics of the two selected trials:  $S_4$  and  $\alpha_4$  are respectively the mean wind horizontal speed and direction at the 4-m level of mast S,  $k_4$  is the turbulent kinetic energy and  $L$  the Monin-Obukhov length at the 4-m level of tower T,  $Q$  is the tracer release rate at the source, ‘Source location’ is the position of the source and  $z_s$  is the height of the source (after Milliez and Carissimo (2007)).

277 paper, trials 2681829 and 2092157 are studied, respectively corresponding to situations of  
 278 neutral and stable atmospheres. The characteristics of these trials are summarized in  
 279 Table 1, and the characteristics of all cases can be found in Milliez and Carissimo (2007).

280 More precisely, the MUST simulations made in different meteorological conditions by  
 281 Milliez and Carissimo (2007) have been reused. These simulations only used the Eulerian  
 282 approach with a  $k - \epsilon$  turbulence closure. In this paper, new  $R_{ij} - \epsilon$  Eulerian and La-  
 283 grangian dispersion simulations are provided within the same calculations so that they can  
 284 be compared with the same Eulerian dynamical field, including the stratification effects. To  
 285 take into account these effects, the code solves for potential temperature, as fully explained  
 286 in Milliez and Carissimo (2007).

287

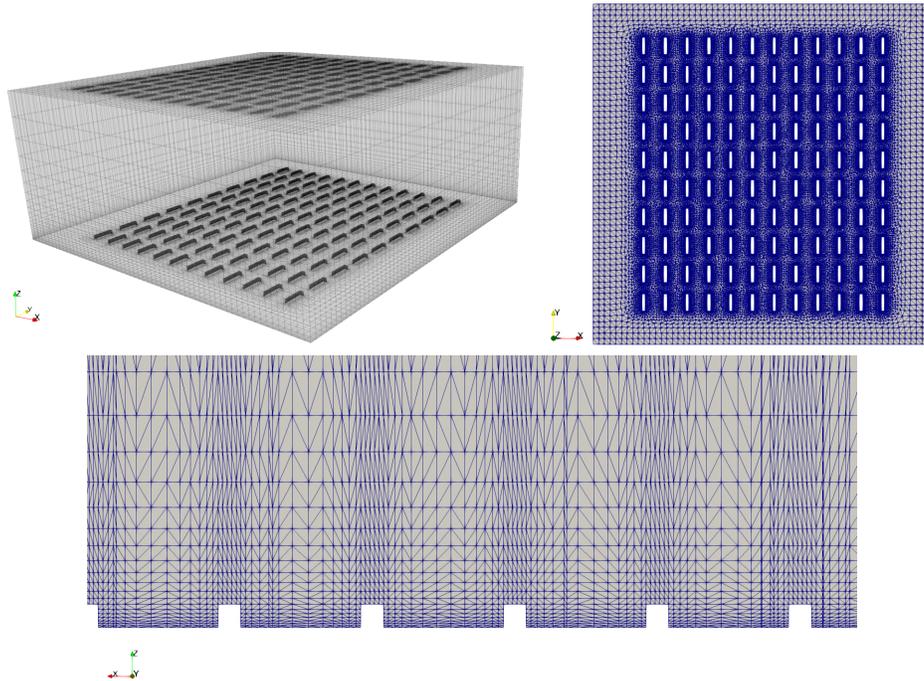


Figure 3: Mesh of the computational domain. From left to right and top to bottom: general view, horizontal cross-section, vertical cross-section.

## 288 4. Numerical simulations

289 In this section, the methodology and results of the numerical simulations of trials  
 290 2681829 and 2692157 in *Code\_Saturne* are presented.

### 291 4.1. Simulation domain and mesh

292 The simulation domain is of dimensions 240 m (North-South)  $\times$  240 m (East-West)  $\times$   
 293 100 m (vertical direction). The corresponding mesh is displayed in Figure 3. It is refined  
 294 near the ground and the obstacles, the horizontal resolution varying from 4 m to 0.6 m.  
 295 The vertical resolution of the mesh increases gradually from 0.2 m near the ground until  
 296 it reaches 4 m at the top of the domain. In total, the mesh contains 1 426 010 cells.

### 297 4.2. Numerical setup

#### 298 4.2.1. Fluid phase

299 For the flow, the models  $k - \epsilon$  et  $R_{ij} - \epsilon$  (with simple gradient-diffusion hypothesis for  
 300 the scalars) are used and will be further compared. The imposed boundary conditions are  
 301 as follows:

- 302 • Inlet condition of Dirichlet type, with dynamical profiles derived from experimen-  
 303 tal measurements. Indeed, it has been shown in Milliez and Carissimo (2007) that

the use of analytical profiles in equilibrium can induce an underestimation of turbulence. They found better results using experimental profiles (when available), which is why we have chosen to follow the same road. More precisely, the TKE profiles are estimated from the available measurements and then the turbulent dissipation rate profiles are deduced from the relations from Monin-Obukhov theory as given in Duynkerke (1988) and reused in Milliez and Carissimo (2007):

$$k = \frac{u_L^2}{\sqrt{C_\mu}}, \quad (5a)$$

$$\epsilon = \frac{u_L^3}{\kappa} \left( \frac{1}{z} + \frac{4}{L} \right), \quad (5b)$$

where  $u_L$  is the local stress equal to  $u_*(1 - z/h)$  where  $h$  is the height of the boundary layer (Stull, 1988) and  $u_*$  the surface stress. Also,  $\kappa$  is the von Karman constant and  $L$  is the Obukhov length.

In the case of the  $R_{ij} - \epsilon$  model, the  $R_{ij}$  tensor at the boundary is given as follows: the diagonal terms are constructed isotropically from the turbulent kinetic energy and the other terms are taken as zero. These are reasonable hypotheses that can be expected in operational use (and similar for both  $k - \epsilon$  and  $R_{ij} - \epsilon$  models). We have verified elsewhere that the model rapidly adjusts to a more realistic  $R_{ij}$  tensor, well before reaching the obstacles.

- Outlet condition: free outflow.
- Ground and containers: rough wall, with a roughness length of 0.04 m. A logarithmic wall function is used. A Dirichlet condition is applied for  $k$ , such that  $k = u_*^2/\sqrt{C_\mu}$  except in the viscous sub-layer where  $k = 0$ . A Neumann condition is applied for  $\epsilon$ , such that  $\epsilon = u_*^3/(\kappa z)$ , except in the viscous sublayer where a zero-flux is imposed.

#### 4.2.2. Dispersed phase

With the Eulerian approach, the pollutant is injected through a scalar source term. At the injection cell, a pollutant flow rate of 225 L/min has been imposed for both neutral 2681829 and stable 2692157 trials (cf. Table 1). With the Lagrangian approach, at the same injection cell, 2000 particles per time step have been injected, with the same flow rate.

### 4.3. Results for neutral trial 2681829

#### 4.3.1. Simulation of the fluid phase

As exposed in the previous section, two simulations of the fluid phase have been performed, corresponding respectively to the use of the  $k - \epsilon$  or second-order  $R_{ij} - \epsilon$  turbulence closures. Figure 4 shows the mean velocity and TKE fields at height  $z = 4$  m for both

335 turbulence models. This height stands above the roofs ( $z_{roofs} = 2.54$  m) and we can ob-  
 336 serve the influence of the row of containers on the flow. Naturally, a slowdown of the flow  
 337 and an increase in turbulent kinetic energy can be observed. It can also be seen that  $k - \epsilon$   
 338 model tends to predict higher levels of turbulent kinetic energy upstream of the obstacles,  
 339 which is a well-known result in turbulence modeling. However, when comparing to the  
 340 measurements, it can be seen that the TKE values are always underestimated, with both  
 341  $k - \epsilon$  and  $R_{ij} - \epsilon$  models. Figure 5 shows the wind field in the source area, at 1.6 m height:  
 342 the recirculation zones between the containers are well-captured and explain the previously  
 343 mentioned decrease of velocity above the roofs at 4 m height. The recirculation zones are  
 344 also wider and more pronounced with the  $R_{ij} - \epsilon$  model. Finally, the mean velocity and  
 345 TKE vertical profiles extracted from the masts have been plotted in Figure 6 when data  
 346 was available. Once again, turbulence production is more pronounced with  $k - \epsilon$  model.  
 347 Velocity profiles are on the other hand not much affected by the turbulence model (as is  
 348 also seen in the velocity magnitude field of Figure 4) and stand in good agreement with  
 349 the measurements.

#### 350 4.3.2. Simulation of the dispersion

351 Figure 7 shows the concentration fields at height 1.6 m, for both  $k - \epsilon$  and  $R_{ij} - \epsilon$  models.  
 352 Whether it be through the Eulerian or the Lagrangian approach, it can be observed that  
 353 the choice of the turbulence model plays an important role on the concentration patterns.  
 354 In particular, it can be seen that the plume is wider using the  $R_{ij} - \epsilon$  model.

355 One can also observe that there is a deflection of the plume centerline compared to  
 356 the  $-41^\circ$  wind direction. Note also that the plume deflection is more pronounced when  
 357 using the  $R_{ij} - \epsilon$  model, for both Eulerian and Lagrangian approaches. This deviation  
 358 phenomenon has also been observed in Carissimo and Macdonald (2004) and Milliez and  
 359 Carissimo (2007). Milliez and Carissimo (2007) explained it by the fact the pollutant is  
 360 channeled into the streets perpendicular to the obstacle array axis, as is also observed in  
 361 the experiment. Castelli et al. (2017), who also performed the same trial Eulerian  $k - \epsilon$   
 362 and Lagrangian calculations within their models RAMS6.0-mod and MicroRMS, noticed  
 363 a lesser pronounced deflection with the Lagrangian modeling. They partly explained it by  
 364 pointing out that their Lagrangian code did not account for the cross-correlation terms  
 365 between the different components of wind velocity fluctuations. This is not the case with  
 366 the model used in the present work since it is based on Pope's SLM, which implies that  
 367 the cross-correlations of the wind velocity fluctuations are included in the mean-pressure  
 368 gradient term of Eq. (4b). This is actually one of the main advantages of this formulation,  
 369 see Bahlali et al. (2018b) for more theoretical details. This may be why, when roughly  
 370 comparing the concentration field obtained by Castelli et al. (2017) to the one displayed  
 371 in Figure 7, a more pronounced deflection is found with the SLM than in Castelli et al.  
 372 (2017)'s results.

373 For a more precise analysis of the concentration field, the concentration horizontal  
 374 profiles on lines 1, 2, 3, 4 are shown in Figure 8, and the vertical profiles on masts B, C, D  
 375 and tower T are displayed in Figure 9. It can be observed that, in particular, the lines 1 and

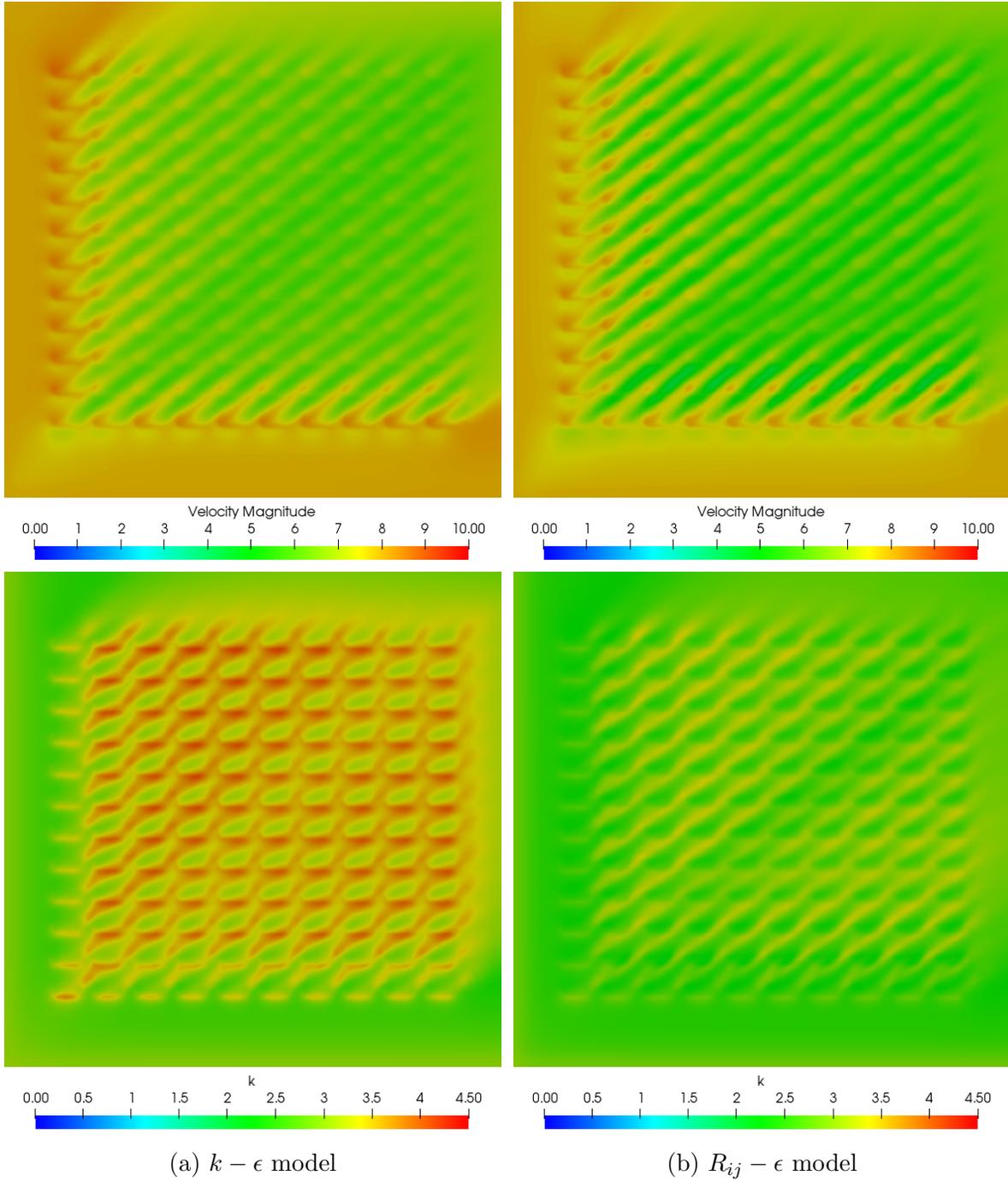


Figure 4: Comparison of mean velocity and TKE fields at  $z = 4$  m computed by  $k - \epsilon$  or  $R_{ij} - \epsilon$  turbulence models, for neutral trial 2681829.

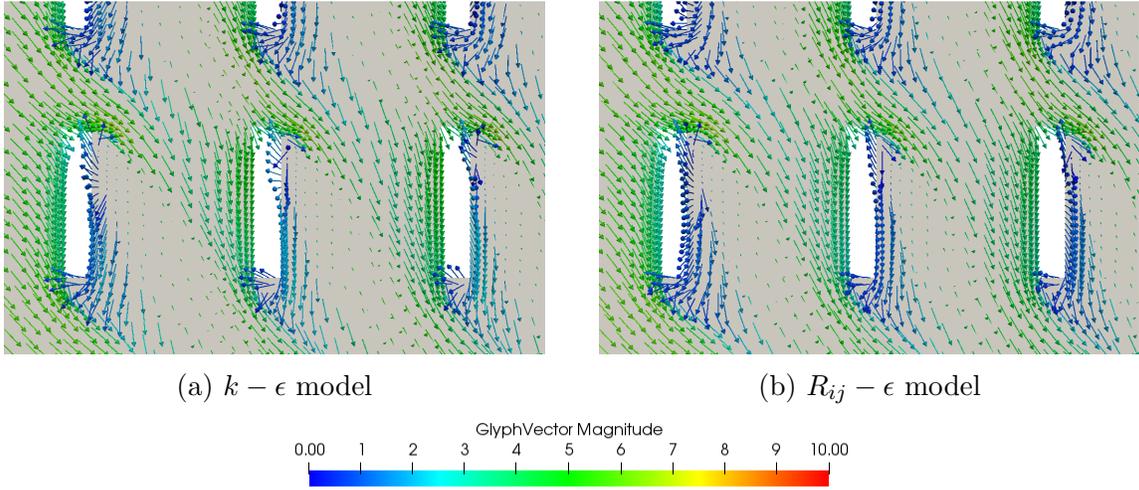


Figure 5: Comparison of wind fields around the source computed by  $k - \epsilon$  or  $R_{ij} - \epsilon$  turbulence models, for neutral trial 2681829.

376 2 show a shift in the plumes obtained by respectively the  $k - \epsilon$  and the  $R_{ij} - \epsilon$  models, which  
 377 again highlights the observed more pronounced deflection with the  $R_{ij} - \epsilon$  closure. When  
 378 using the  $R_{ij} - \epsilon$  closure, the effect of the obstacles is clearly visible through the ‘steps’  
 379 corresponding to the regular spacing between the containers. If one compares Eulerian to Lagrangian  
 380 results, it is interesting to have a look at the concentration evolution from  
 381 line 1 (closest to the source) to line 4. Both models seem to have approximately the same  
 382 evolution of diffusion. This is better seen in Figure 10, where the maximum concentration  
 383 value over each line against the distance from the source has been plotted. It is well-  
 384 known that Langevin-like Lagrangian models show rapid diffusion near the source and  
 385 then tend to follow the diffusive law in the far-field. On the other hand, Eulerian models  
 386 based on a simple gradient diffusion hypothesis portray the whole dispersion process by  
 387 the diffusive law (which is actually a shortcoming of this kind of models since the gradient-  
 388 diffusion hypothesis is no longer valid near the source). One then might wonder why, here  
 389 in Figure 10, both Eulerian and Lagrangian models seem to show the same evolution of  
 390 diffusion, independently from the distance to the source. In fact, one important thing to  
 391 point out here is that line 1 is already located in the so-called ‘far-field region’. Indeed,  
 392 when speaking about near and far fields, it is always in comparison to the value of the  
 393 Lagrangian integral timescale  $T_L$ . For small diffusion times with respect to the value of  
 394  $T_L$ , diffusion should be evolving proportionally to time, while for higher diffusion times, it  
 395 should be evolving as square-root of time (Taylor, 1921). In the present case, the value of  
 396  $T_L$  at the injection cell is 0.93 s, and the velocity norm is  $4.5 \text{ m.s}^{-1}$ , which yields a ‘near-field  
 397 region’ of approximately  $0.93 \times 4.5 = 4.2 \text{ m}$ . The far field is thus quickly reached. As the  
 398 maximum concentration value on line 1 is located at approximately 60 m ( $\gg 4.2 \text{ m}$ ) from  
 399 the source, we deduce by extension that all the lines are already in the well-established far-  
 400 field region. In consequence, it is only logical that both the Lagrangian and the Eulerian  
 401 models show the same evolution of diffusion.

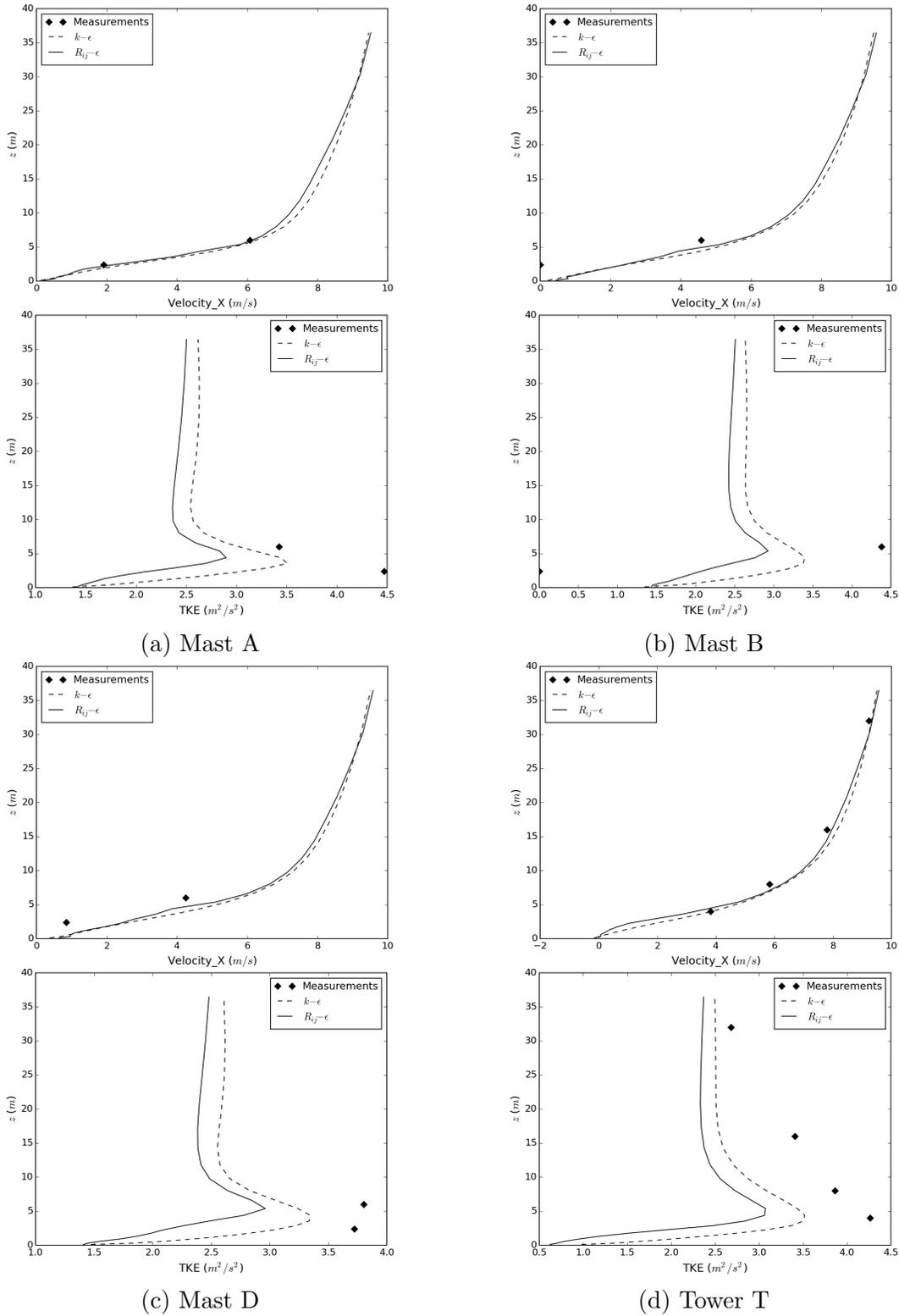


Figure 6: Comparison of vertical velocity and TKE profiles computed by  $k-\epsilon$  or  $R_{ij}-\epsilon$  turbulence models, for neutral trial 2681829.

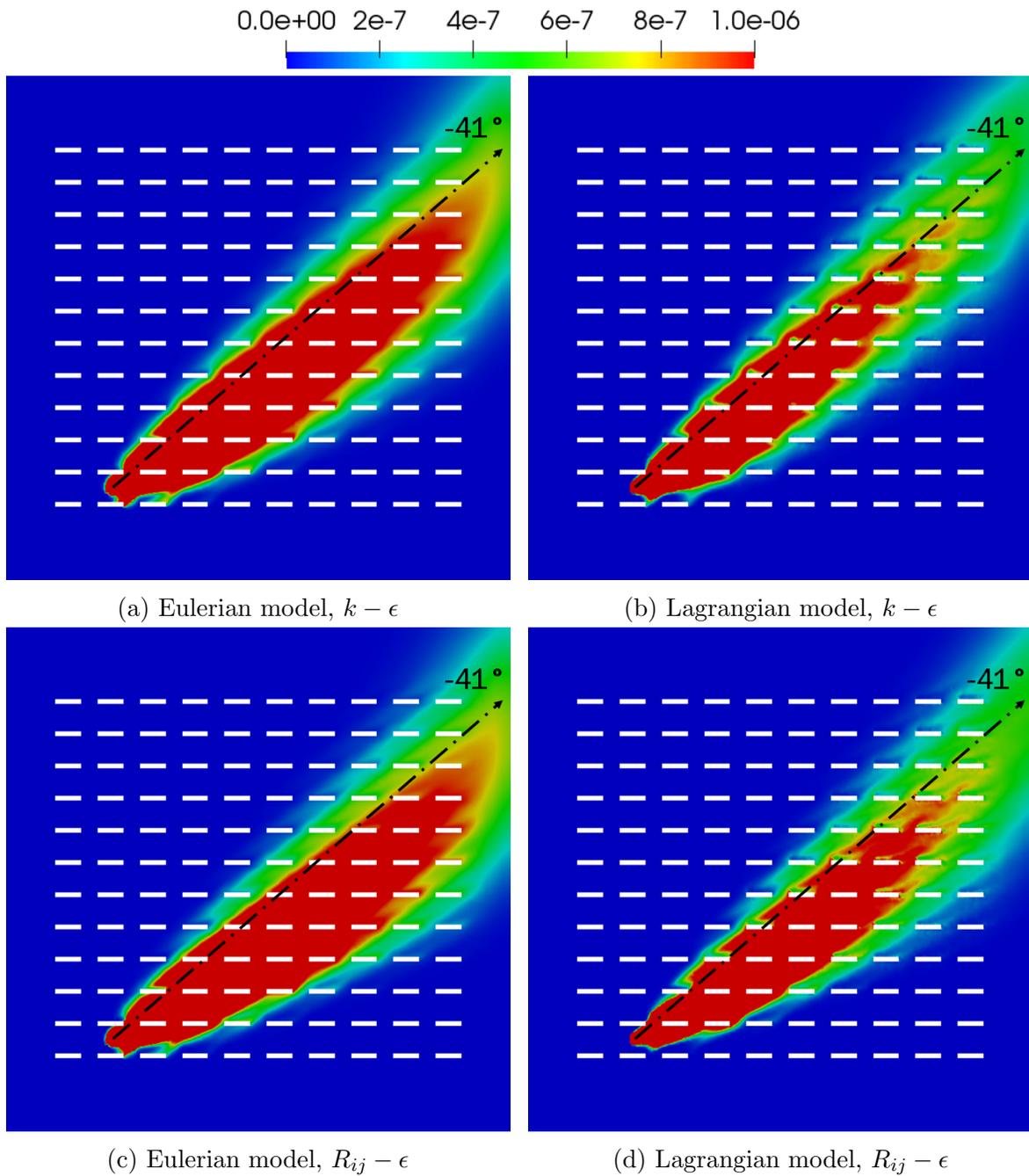


Figure 7: Comparison of mean concentration ( $kg/kg$ ) fields at  $z = 1.6$  m computed by both Eulerian and Lagrangian models, through  $k - \epsilon$  or  $R_{ij} - \epsilon$  turbulence closures, for neutral trial 2681829.

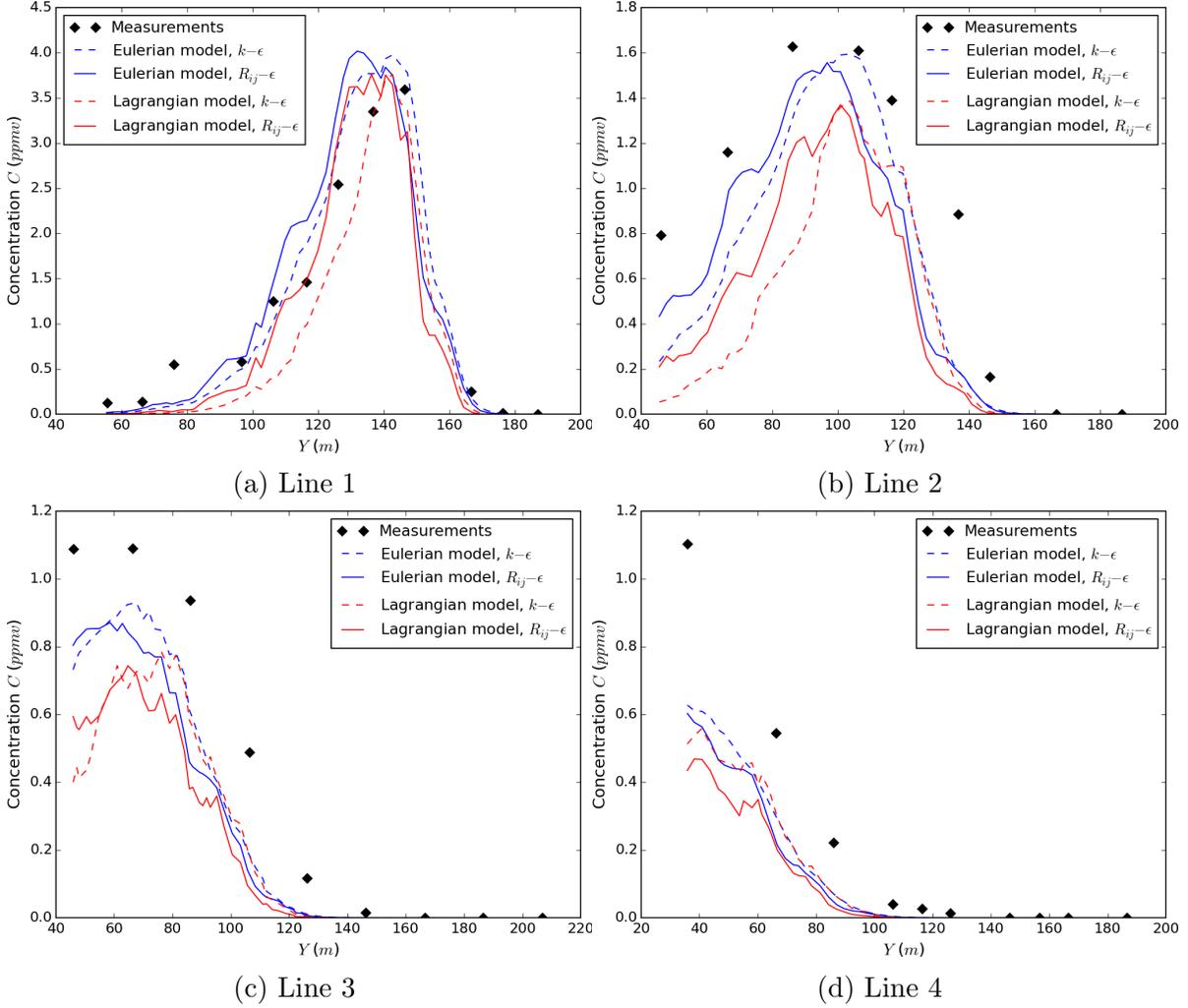


Figure 8: Comparison of concentration profiles on horizontal line samplers computed by both Eulerian and Lagrangian models, through  $k - \epsilon$  or  $R_{ij} - \epsilon$  turbulence closures, for neutral trial 2681829.

402 Apart from the previous remarks, and still analyzing the lines, the agreement between  
 403 simulations and measurements is overall satisfactory and both Eulerian and Lagrangian  
 404 models provide a quite acceptable representation of the spread of the plume, although the  
 405 Lagrangian model seems to slightly underestimate the concentrations on all the lines.

406 If we focus now on vertical profiles (see Figure 9), it can be seen that the use of the  
 407  $R_{ij} - \epsilon$  model for the fluid phase tends to reduce the maxima of concentrations on mast  
 408 B (closest to the source), especially with the Lagrangian approach, making the results in  
 409 better agreement with the measurements. On tower T, the maxima of concentrations are  
 410 also lower and are due to the fact that the plume deflection is more pronounced using the  
 411  $R_{ij} - \epsilon$  model for both Eulerian and Lagrangian approaches, making the plume go towards  
 412 the South direction with more intensity and leaving lower concentration values on tower T.  
 413 On mast C, the concentrations are also slightly reduced when using the  $R_{ij} - \epsilon$  model for

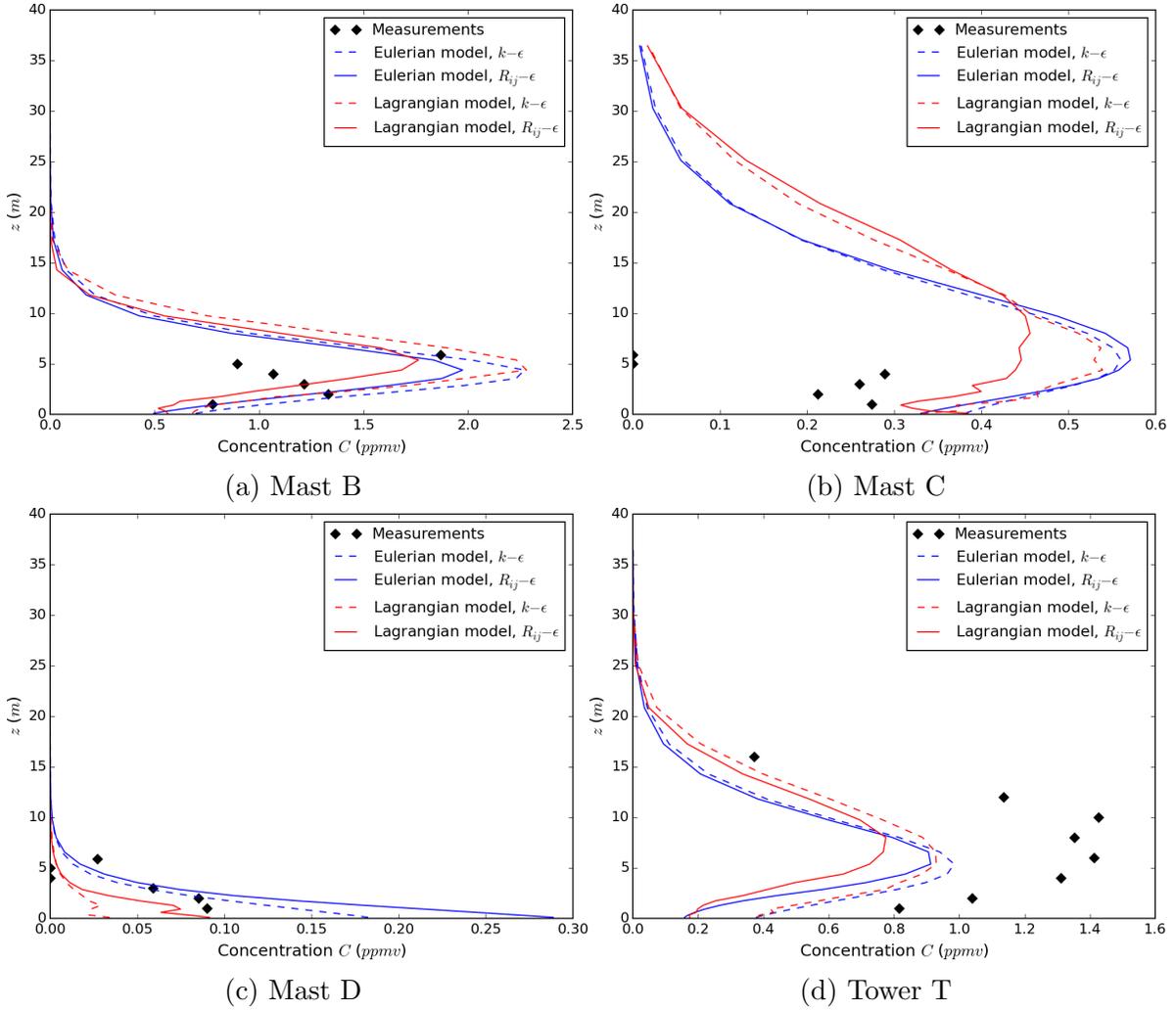


Figure 9: Comparison of vertical concentration profiles computed by both Eulerian and Lagrangian models, through  $k-\epsilon$  or  $R_{ij}-\epsilon$  turbulence closures, for neutral trial 2681829.

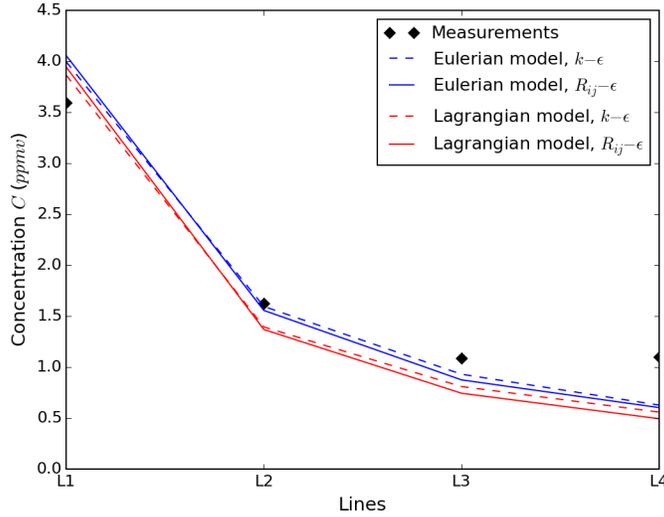


Figure 10: Maximum concentration value over each line against the distance from the source, for neutral trial 2681829.

414 the same reason as for tower T. It is interesting to **note** that on this mast, the Lagrangian  
 415 approach captures the change of sign in the vertical gradient of concentration near the  
 416 ground, while the Eulerian model does not. This is even more marked with the use of the  
 417  $R_{ij} - \epsilon$  model. Finally, on mast D, concentrations are raised up when using the  $R_{ij} - \epsilon$   
 418 model, which can also be explained by the plume deflection towards the South direction  
 419 more pronounced with this model. On this mast, the Lagrangian approach provides better  
 420 agreement with the measurements. However, note that one must be cautious in giving  
 421 definite conclusions for masts C and D, since the concentrations are lower and can then  
 422 imply more significant errors and uncertainties.

#### 423 4.4. Results for stable trial 2692157

##### 424 4.4.1. Simulation of the fluid phase

425 Analogously to neutral trial 2681829, we show in Figure 11 the mean velocity and TKE  
 426 vertical profiles on masts A, B, C and tower T for both  $k - \epsilon$  and  $R_{ij} - \epsilon$  turbulence models.  
 427 Velocities and TKE values are much lower than for trial 2681829, which is typical of stable  
 428 stratification meteorological conditions. As in case 2681829,  $k - \epsilon$  model tends to predict  
 429 higher values of TKE than does  $R_{ij} - \epsilon$  model. Velocity profiles are in good agreement with  
 430 the measurements. Once again, they are not much affected by the choice of the turbulence  
 431 model.

##### 432 4.4.2. Simulation of the dispersion

433 Figure 12 displays the different concentration fields at height 1.6 m. It can be seen that  
 434 as in trial 2681829, the plume is also wider when  $R_{ij} - \epsilon$  model is used. The difference is  
 435 even more pronounced through the Lagrangian approach. In addition, a plume deflection  
 436 (compared to the  $43^\circ$  wind direction) can also be observed in both Eulerian and Lagrangian

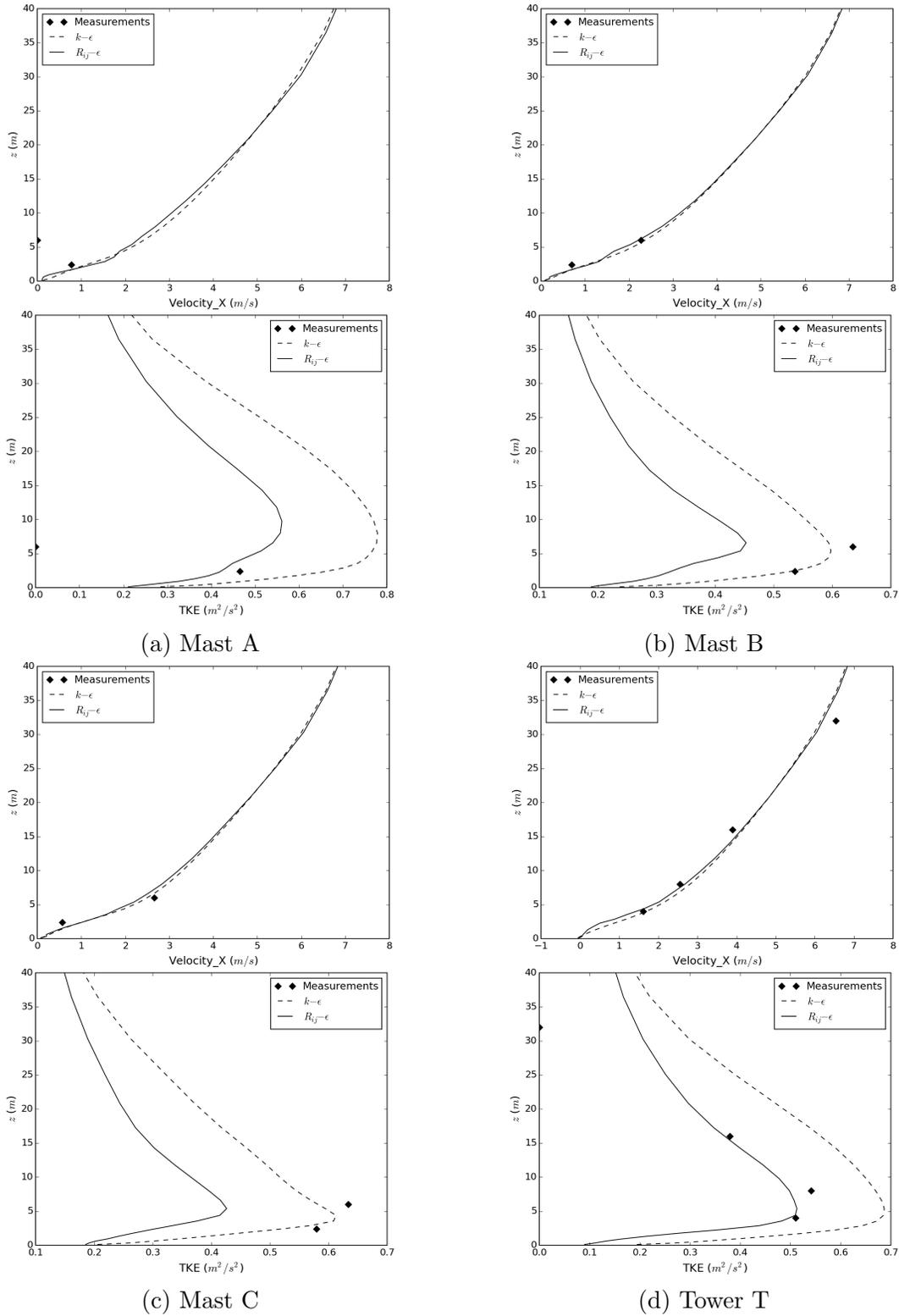


Figure 11: Comparison of vertical velocity and TKE profiles computed by  $k-\epsilon$  or  $R_{ij}-\epsilon$  turbulence models, for stable trial 2692157.

437 results, more significant when using the  $R_{ij} - \epsilon$  than the  $k - \epsilon$  model for the fluid phase  
438 computation.

439 The horizontal concentration profiles on lines 1, 2, 3 and 4 are shown in Figure 13. It  
440 can be seen that the use of the  $R_{ij} - \epsilon$  model leads to an overprediction of concentrations  
441 on line 1, for both Eulerian and Lagrangian approaches, even more marked on the Eulerian  
442 results. Such an overprediction may be due to the fact that TKE is underestimated with  
443 the  $R_{ij} - \epsilon$  model as seen in Figure 11. Nevertheless, the  $R_{ij} - \epsilon$  model shows again the  
444 advantage of better capturing the presence of the obstacles through the visible regular  
445 concentration ‘steps’. Regardless of the turbulence model, one can also notice the strong  
446 decrease of concentrations between line 1 and line 2 with both Lagrangian and Eulerian  
447 models, less marked when moving to the next lines: the evolution of diffusion induced by  
448 both models look similar. In this trial, at the injection cell,  $T_L = 0.73$  s and the velocity  
449 equals  $1.7$  m.s<sup>-1</sup>: in consequence, the region corresponding to the ‘near field’ corresponds to  
450 distances below  $0.73 \times 1.7 = 1.2$  m. The far field is thus immediately reached. Finally, one  
451 may notice that the larger the distance from the source, the closer Eulerian and Lagrangian  
452 curves approach each other. Also, the agreement with experimental measurements is much  
453 better.

454 The vertical concentration profiles on masts A, B, D and tower T are displayed in  
455 Figure 14. On mast D, which is the closest to the source, both Lagrangian and Eulerian  
456 models overpredict the concentrations when the  $R_{ij} - \epsilon$  model is used. Nevertheless, when  
457 using the  $k - \epsilon$  closure, both models provides very accurate results. Same goes for tower  
458 T, where the use of the  $R_{ij} - \epsilon$  turbulence closure leads to an overprediction of concen-  
459 tration especially near the ground. On this mast, it is interesting to point out that even  
460 though the Lagrangian model used with the  $k - \epsilon$  closure underpredicts the concentration  
461 values, it captures the change in the sign of the vertical concentration gradient near the  
462 ground. Stepping even further from the source and looking at mast A, one can notice a  
463 stronger vertical diffusion in the Lagrangian results. In this case again, concentrations are  
464 overpredicted. For this trial, the study of masts D, T and A is interesting as the ‘D-T-A’  
465 parametrical line is roughly aligned with the centerline of the plume. One general conclu-  
466 sion from these three masts is that the use of the  $R_{ij} - \epsilon$  model leads to an overprediction  
467 of concentrations especially near the ground. As for the concentrations on mast B, they  
468 are influenced by the plume deviation. Indeed, since the  $R_{ij} - \epsilon$  model involves a more  
469 pronounced deflection of the plume than the  $k - \epsilon$  model towards the West direction, where  
470 mast B is located, then concentrations are expected to be higher, which is indeed what  
471 is observed in the simulation results. However, and once again, better accuracy is found  
472 when the  $k - \epsilon$  model is used for both Eulerian and Lagrangian approaches (except on  
473 mast B for the Lagrangian results).

474 From all these results on stable stratification, one may think that the tendency of  
475 the  $k - \epsilon$  model to compute high TKE values can be seen as an ‘advantage’ for stable  
476 conditions, since this strengthens diffusion processes and thus leads to lower concentration  
477 values (that are, in general, and in particular looking at the lines, in better agreement with  
478 the measurements). In fact, one should remember here that even when using a  $R_{ij} - \epsilon$

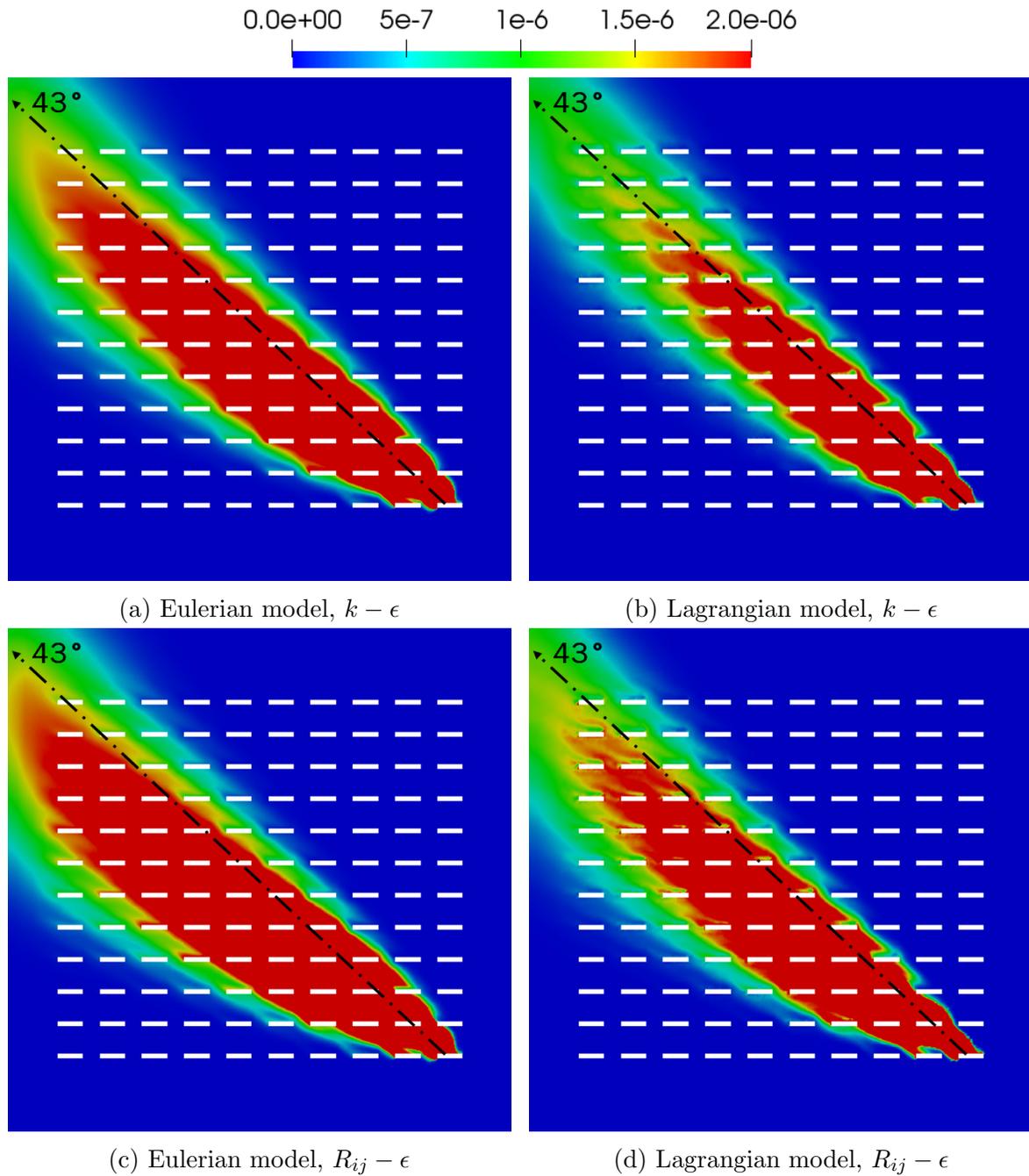


Figure 12: Comparison of mean concentration ( $kg/kg$ ) fields at  $z = 1.6$  m computed by both Eulerian and Lagrangian models, through  $k - \epsilon$  or  $R_{ij} - \epsilon$  turbulence closures, for stable trial 2692157.

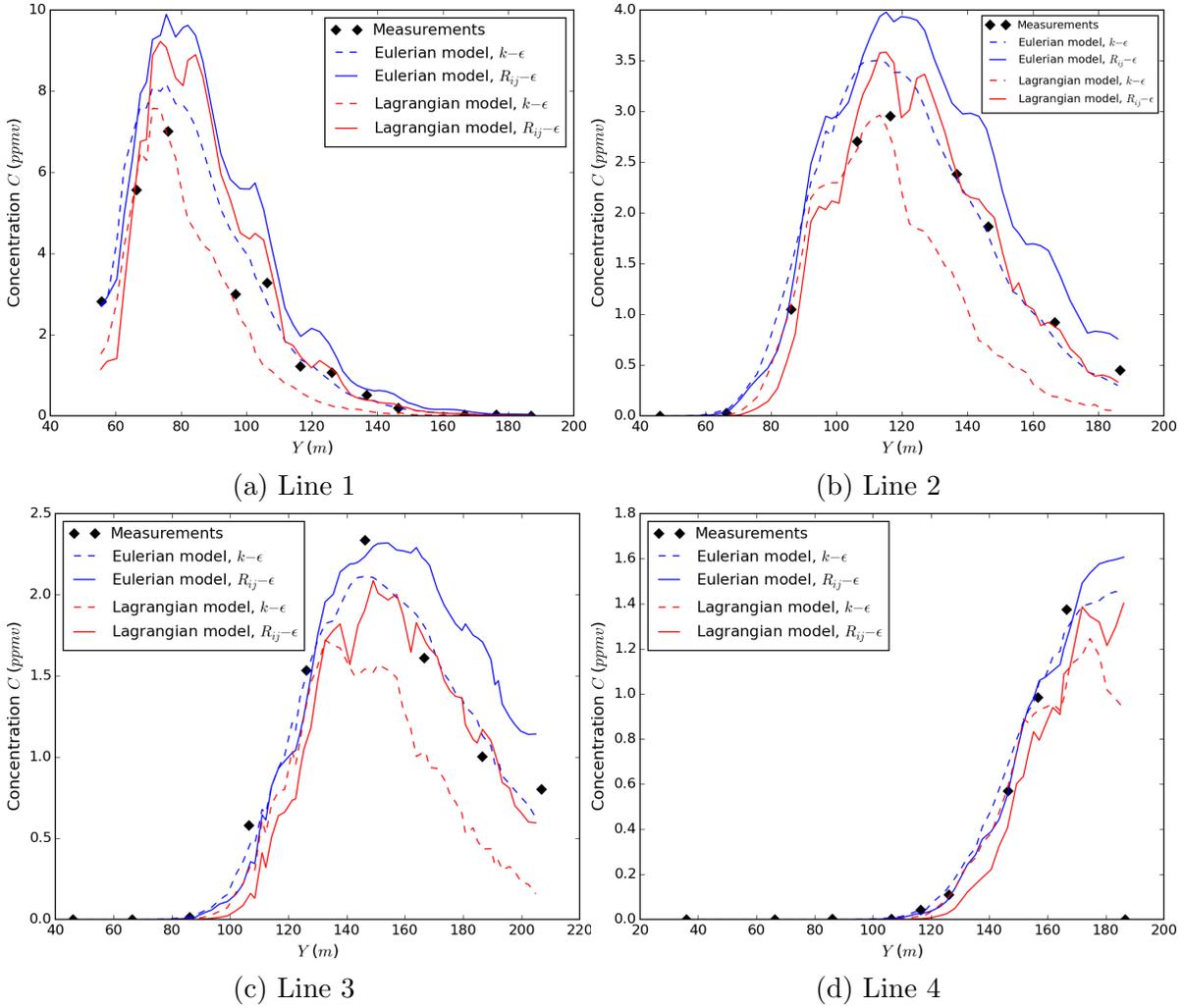


Figure 13: Comparison of concentration profiles on horizontal line samplers computed by both Eulerian and Lagrangian models, through  $k-\epsilon$  or  $R_{ij}-\epsilon$  turbulence closures, for stable trial 2692157.

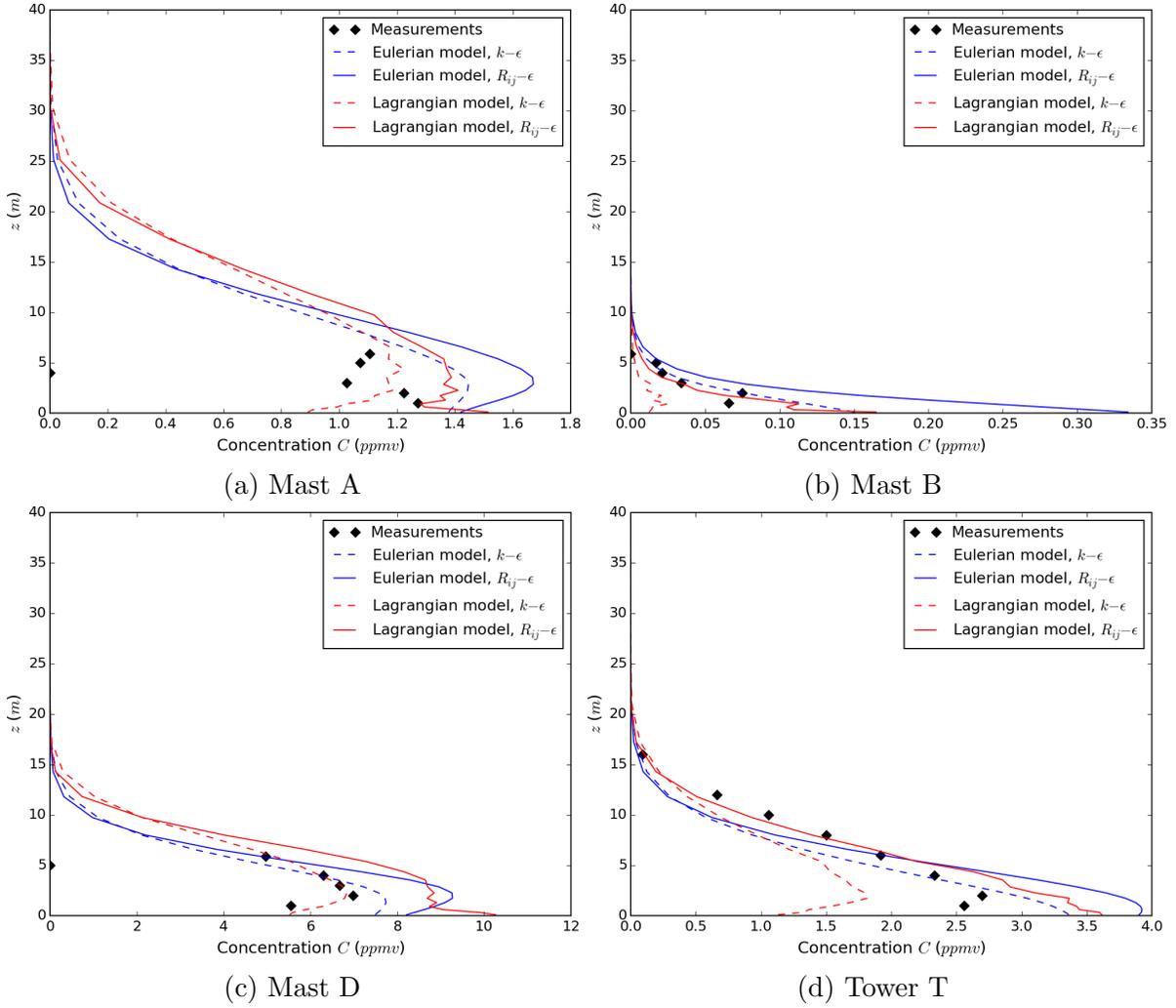


Figure 14: Comparison of vertical concentration profiles computed by both Eulerian and Lagrangian models, through  $k - \epsilon$  or  $R_{ij} - \epsilon$  turbulence closures, for stable trial 2692157.

479 model, the closure on potential temperature is still local, through the following Generalized  
 480 Gradient Diffusion Hypothesis (GGDH):

$$\langle U'_{f,j} \theta' \rangle = -C_\theta \frac{k}{\epsilon} \left( \langle U'_{f,j} U'_{f,k} \rangle \frac{\partial \langle \theta \rangle}{\partial x_k} \right), \quad (6)$$

481 where  $C_\theta = 0.3$ .

482 An improvement, still under investigation, could be the use of a second-order model on  
 483 potential temperature.

## 484 5. Conclusions

485 This work aimed at assessing the ability of a Lagrangian stochastic model to perform  
 486 point source dispersion in an idealized urban area, for neutral and stable meteorological  
 487 conditions. The Lagrangian model used was a model based on Pope (2000)'s SLM and  
 488 Minier and Peirano (2001)'s two-phase flow formulation. Pope's PDF models have gone  
 489 quite unnoticed in the atmospheric dispersion community, despite presenting some non-  
 490 negligible theoretical and numerical advantages (see Bahlali et al. (2018a,b)).

491 As used within a hybrid Eulerian/Lagrangian approach, the Lagrangian solver was  
 492 fed by the mean dynamical fields provided by the Eulerian solver of the same CFD code  
 493 *Code\_Saturne*. These fields were computed either through a  $k - \epsilon$  model or a second-order  
 494  $R_{ij} - \epsilon$  model. The Lagrangian results were compared to the Eulerian ones, for both  
 495 turbulence models. The Eulerian turbulence closure for the scalar fluctuations was **based**  
 496 **on the gradient-diffusion hypothesis**, which implied constant diffusivity. We showed that  
 497 since the region considered for concentration measurements is already located in the far  
 498 field (*i.e.*, diffusion times higher than the Lagrangian integral timescale), both Eulerian  
 499 and Lagrangian show the same evolution of diffusion.

500 Then, we showed that the obstacle array induced a deflection of the plume, as already  
 501 observed by Milliez and Carissimo (2007) in the same code and Castelli et al. (2017) in  
 502 another methodology. These works modeled turbulence only through a  $k - \epsilon$  closure. **More**  
 503 **precisely**, we showed that this plume deflection was more pronounced using a  $R_{ij} - \epsilon$   
 504 model. This was the case with both Eulerian and Lagrangian approaches. For neutral  
 505 stratification, the agreement between results and measurements is quite satisfactory. In  
 506 particular, we can validate the accuracy of the results of the Lagrangian model. We showed  
 507 that the use of the  $R_{ij} - \epsilon$  model made it possible to have a more physical representation  
 508 of the obstacles' influence on the concentration profiles, through the visible regular 'steps'  
 509 corresponding to the spacing between the containers.

510 For stable stratification, we showed that the results obtained by both approaches were  
 511 more accurate when using a  $k - \epsilon$  closure for the fluid phase. Not as satisfactory results as  
 512 for neutral trial were found with the use of the  $R_{ij} - \epsilon$  closure for stable stratification. The  
 513 Lagrangian model, which is dependent on the quality of the flow calculated by the Eulerian  
 514 solver, also see its results affected by the use of the  $R_{ij} - \epsilon$  model. Deeper investigations are

515 needed on this subject, as it should be noted that the temperature and scalar fluctuations  
516 closures are still local even when using the  $R_{ij} - \epsilon$  model.

517 It is worth noting that the differences between the various results shown in this pa-  
518 per can be interpreted in different ways. In a practical context where order of magnitude  
519 differences are expected, they can be seen as small. On the other hand, they can also be  
520 looked at as an estimate we can have on the uncertainty effects of adopting either a certain  
521 turbulence closure ( $k - \epsilon$  or  $R_{ij} - \epsilon$ ) or one of the two Lagrangian or Eulerian approaches.

522 For further investigations, an idea would be to explore full second-moment closure mod-  
523 eling for both temperature and scalar fluctuations. In the Lagrangian modeling, another  
524 research path would be to add a temperature scalar to the state vector of the particles,  
525 driven by a new stochastic differential equation (in the spirit of the works of Das and Durbin  
526 (2005) or Bossy et al. (2018) for instance), in order to better account for buoyancy-induced  
527 turbulent patterns.

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