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Comparison of two turbulence parameterisations for the simulation of the concentration variance dispersion

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Abstract
In this work, we compare two different parameterisations for the wind velocity–component standard deviations. The first one is the (Hanna 1982) parameterisation, while the second is the (Scire et al. 2000) parameterisation, which provide the proper values and vertical structure for the wind standard deviations in the convective, neutral and stable layers, needed as input the Lagrangian stochastic model SPRAYWEB. The results of the model simulations carried out using the two parameterisations are compared, in terms of both mean concentration and concentration standard deviation, by evaluating some statistical indexes and trough scatter- and qq-plots.

Keywords Lagrangian model · Turbulence parameterisation · Tracer experiment

Introduction

Concentration variance–field simulation model's development began around the late 1950s (Hinze 1959), and different approaches have been tried since then. The most relevant are the *Fluctuating Plume* (Gifford 1959; Franzese and Borgas 2002; Franzese 2003; Yee et al. 2003; Gailis et al. 2007; Mortarini et al. 2009; Ferrero et al. 2013) and the *Two-Particle* models (Durbin 1980; Thomson 1990; Ferrero and Mortarini 2005; Mortarini and Ferrero 2005). However, both models have their drawbacks. *Fluctuating Plume* models provide a good approximation close to the source, but they fail at larger distances, while *Two-Particle* models are able to simulate concentration fields only in idealized atmosphere conditions, and they have some limitations in real atmosphere. For a complete review, see (Ferrero et al. 2020).

We follow the approach of Manor (2009) that proposed a single-particle Lagrangian stochastic model, that analyses the dispersion phenomena following a large number of particles from their source along their Lagrangian trajectory, with every particle motion being independent from the others. Despite being a Lagrangian model, concentrations are evaluated on fixed grid points in a computational domain, like Eulerian models.

We applied a simplified version of the model for simulating the FFT-07 tracer experiment (Storwald 2007; Platt et al. 2008), and later on, we tested the SPRAYWEB model (Tinarelli et al. 1994; Alessandrini and Ferrero 2009; Bisignano et al. 2016; Tomasi et al. 2019) against the same data set. In that work, we use the Hanna parameterisation. In the present work, we compare this parameterisation with those due to Scire et al. (Scire et al. 2000).

The model and the field experiment used for the intercomparison are described in "The numerical model". "Results" is devoted to the results. In "Discussion and conclusions", the main conclusions are discussed.

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The numerical model

SPRAYWEB

The SPRAYWEB model is a 3D purely Lagrangian stochastic particle model which is designed to take into account the spatial and temporal variability of both the meteorological mean flow and turbulence. The model can simulate time-varying emissions from point, area and line sources. SPRAYWEB is particularly suitable for applications over complex terrain, where the meteorological fields are characterized by local phenomena, which introduce great spatial (and temporal) inhomogeneity. Indeed, the model simulates the emitted plume with a great number of virtual particles characterized by a (small) pollutant mass, which passively follows the turbulent motion of the input meteorological field. The mean trajectory of each particle is driven by the local mean wind field (given as input to the model), while its dispersion is determined by turbulent velocities obtained by solving the Langevin stochastic differential equations (Thomson 1987), using the statistical characteristics of the atmospheric turbulence.

An expression for the source Q_v(r) of the concentration variance $\overline{c^2}$, where c is the concentration fluctuation, can be prescribed by observing the Reynolds-averaged equation (RAE) for concentration variance, in which a source term appears (Manor 2009):

$$Q_v\ (\mathrm{r}) = 2\sigma_i^2 T_{L_i}\left(\frac{\partial \overline{C}}{\partial x_i}\right)^2 \quad (1)$$

where $\sigma_i = \sigma_u, \sigma_v, \sigma_w$; $T_{L_i} = T_{L_u}, T_{L_v}, T_{L_w}$ are the three components of the Lagrangian time scale, $\overline{C}(x, y, z, t)$ is the mean concentration and the Einstein notation is assumed.

Following (Manor 2009; Ferrero et al. 2017), the concentration variance dissipation can be expressed with an exponential decay formula:

$$\frac{d\overline{c^2}}{dt} = -\frac{\overline{c^2}}{t_d} \quad (2)$$

where the term $t_d(z)$ is the *decay time scale*. As far as velocity standard deviations and Lagrangian time scale are concerned, the widely used parameterisations (Hanna 1982) are tested; while as for the decay time parameterisation, we follow (Ferrero et al. 2017).

The turbulence parameterisations

In this work, we compare two different parameterisations for the wind velocity component standard deviations. The first one is the Hanna (Hanna 1982) parameterisation, while the second is the Scire et al. (Scire et al. 2000) parameterisation, which provide the proper values and vertical structure for the wind standard deviations in the convective, neutral and stable layers and for intermediate conditions, without physically unrealistic discontinuities. Standard deviations of the wind velocity components are calculated on the basis of the surface-layer (SL) scales. For the SPRAYWEB model, a dedicated WRF/SPRAYWEB Interface [here- after WSI: 21, 22] was developed and implemented to allow the transfer of the WRF output onto the dispersion model. As a matter of fact, the Weather Research Forecast (WRF, (Skamarock and Klemp 2008)) model is used to drive the SPRAYWEB. It is worth mentioning that among the available option for the planetary boundary layer (PBL) model in WRF, we use the YSU scheme. In WSI, two alternative parameterisations for the calculation of the wind standard deviations are implemented. The well-known Hanna (Hanna 1982) parameterisation calculates the values of wind standard deviations and Lagrangian time scales as functions of the SL scales. These relations are based on the analysis of data from field experiments (Hanna 1968, 1981; Kaimal et al. 1976; Caughey et al. 1979), theoretical considerations (Panofsky et al. 1977; Irwin 1979) and a second-order closure model (Wyngaard and Cot́ e 1974).

- Convective boundary layer ($L < 0$):

$$\sigma_{u,v} = u_*\left(12 + 0.5\frac{H_{\mathrm{mix}}}{|L|}\right)^{\frac{1}{3}} \quad (3)$$

$$T_{L_{u,v}} = 0.15\frac{H_{mix}}{\sigma_u} \quad (4)$$

- Surface layer $\left(z \leq 0.03\, H_{\mathrm{mix}}\right)$

$$\sigma_w = 0.96\, w_*\left(3\frac{z}{H_{\mathrm{mix}}} - \frac{L}{H_{\mathrm{mix}}}\right)^{\frac{1}{3}} \quad (5)$$

- Mixed layer $\left(0.03\, H_{\mathrm{mix}} < z < 0.4\, H_{\mathrm{mix}}\right)$

$$\sigma_w = \min\left[0.96\, w_*\left(3\frac{z}{H_{mix}} - \frac{L}{H_{mix}}\right)^{\frac{1}{3}}, 0.763\, w_*\left(\frac{z}{H_{\mathrm{mix}}}\right)^{0.175}\right] \quad (6)$$

- Entrainment layer $\left(0.4\, H_{\mathrm{mix}} < z < 0.96\, H_{\mathrm{mix}}\right)$

$$\sigma_w = 0.722\, w_*\left(1 - \frac{z}{H_{\mathrm{mix}}}\right)^{0.207} \quad (7)$$

- Entrainment layer $\left(0.96\, H_{\mathrm{mix}} < z < H_{\mathrm{mix}}\right)$

$$\sigma_w = 0.37\,w_* \tag{8}$$

For the Lagrangian time scales on the vertical direction:

- $(z < 0.1\,H_{\mathrm{mix}})$ and $(z < -L)$

$$T_{L_w} = 0.1\,\frac{z}{\sigma_w}\,\frac{1}{0.55 + 0.38\frac{z}{L}} \tag{9}$$

- $(z < 0.1\,H_{\mathrm{mix}})$ and $(z > -L)$

$$T_{L_w} = 0.59\,\frac{z}{\sigma_w} \tag{10}$$

- $(z > 0.1\,H_{\mathrm{mix}})$

$$T_{L_w} = 0.15\,\frac{H_{\mathrm{mix}}}{\sigma_w}\left(1 - \exp\left[\frac{-5\,z}{H_{\mathrm{mix}}}\right]\right) \tag{11}$$

- Stable boundary layer $(L > 0)$:

$$\sigma_u = 2\,u_*\left(1 - \frac{z}{H_{\mathrm{mix}}}\right) \tag{12}$$

$$\sigma_{v,w} = 1.3\,u_*\left(1 - \frac{z}{H_{\mathrm{mix}}}\right) \tag{13}$$

$$T_{L_u} = 0.15\,\frac{H_{\mathrm{mix}}}{\sigma_u}\left(\frac{z}{H_{\mathrm{mix}}}\right)^{0.5} \tag{14}$$

$$T_{L_v} = 0.07\,\frac{H_{\mathrm{mix}}}{\sigma_v}\left(\frac{z}{H_{\mathrm{mix}}}\right)^{0.5} \tag{15}$$

$$T_{L_w} = 0.10\,\frac{H_{\mathrm{mix}}}{\sigma_W}\left(\frac{z}{H_{\mathrm{mix}}}\right)^{0.8} \tag{16}$$

- Neutral boundary layer $(L \to \infty)$:

$$\sigma_u = 2\,u_*\,\exp\left[-\frac{3f_z}{u_*}\right] \tag{17}$$

$$\sigma_{v,w} = 1.3\,u_*\,\exp\left[-\frac{2f_z}{u_*}\right] \tag{18}$$

$$T_{L_{u,v,w}} = \frac{0.5\,\frac{z}{\sigma_w}}{1 + 15\frac{f_z}{u_*}}, \tag{19}$$

where L is the Obukhov length, H_{mix} is the PBL height, f_z is the Coriolis parameter, u_* is the friction velocity and w_* is the convective velocity scale.

The Scire et al. (Scire et al. 2000) formulation results from a combination of different empirical relations and theoretical reasonings from Panofsky et al. (1977); Hicks 1985; Arya 1984; Blackadar and Tennekes 1968; Nieuwstadt 1984; Hanna et al. 1986). Standard deviations of the flow field are calculated on the basis of the surface-layer scales as follows:

- Convective boundary layer $(L < 0)$:

$$\sigma_{u,v} = \left[4\,u_*^2\,a_n^2 + 0.35\,w_*^2\right]^{\frac{1}{2}} \tag{20}$$

- Surface layer $(z \leq 0.1\,H_{\mathrm{mix}})$

$$\sigma_w = \left[1.6\,u_*^2\,a_n^2 + 2.9\,u_*^2\left(-\frac{z}{L}\right)^{\frac{2}{3}}\right]^{\frac{1}{2}} \tag{21}$$

$$a_n = \exp\left[-0.9\left(\frac{z}{H_{\mathrm{mix}}}\right)\right] \tag{22}$$

- Mixed layer $(0.1\,H_{\mathrm{mix}} < z \leq 0.8\,H_{\mathrm{mix}})$

$$\sigma_w = \left[1.15\,u_*^2\,a_n^2 + 0.35\,w_*^2\right]^{\frac{1}{2}} \tag{23}$$

- Entrainment layer $(0.8\,H_{\mathrm{mix}} < z \leq H_{\mathrm{mix}})$

$$\sigma_w = \left[1.15\,u_*^2\,a_n^2 + a_{cl}\,0.35\,w_*^2\right]^{\frac{1}{2}} \tag{24}$$

$$a_{cl} = \left[\frac{1}{2} + \frac{H_{\mathrm{mix}} - z}{0.4\,H_{\mathrm{mix}}}\right] \tag{25}$$

- Entrainment layer $(H_{\mathrm{mix}} < z \leq 1.2\,H_{\mathrm{mix}})$

$$\sigma_w = \left[1.15\,u_*^2\,a_n^2 + a_{c2}\,0.35\,w_*^2\right]^{\frac{1}{2}} \tag{26}$$

$$a_{c2} = \left[\frac{1}{3} + \frac{1.2\,H_{\mathrm{mix}} - z}{1.2\,H_{\mathrm{mix}}}\right] \tag{27}$$

- Neutral-stable boundary layer $(L \to \infty)$, $(L > 0)$:

$$\sigma_{u,v} = u_*\left[\frac{1.6\,C_s\frac{z}{L} + 1.8\,a_n}{1 + \frac{z}{L}}\right] \tag{28}$$

$$\sigma_w = 1.3\,u_*\left[\frac{C_s\frac{z}{L} + a_n}{1 + \frac{z}{L}}\right] \tag{29}$$

$$C_s = \left(1 - \frac{z}{H_{\mathrm{mix}}}\right)^{\frac{3}{4}} \tag{30}$$

Comparing the two parameterisations, it can be observed that in the case of unstable conditions, for the vertical component of the velocity standard deviation, both of them divide the PBL into different sub-layers and use the surface-layer parameters and the PBL height. Concerning the horizontal components, the Hanna (Hanna 1982) parameterisation uses L and H_{mix}, while the Scire et al. (Scire et al. 2000) parameterisation uses w_*. Also, Scire et al. (Scire et al. 2000) prescribe the same parameterisation for neutral and stable conditions while the Hanna (Hanna 1982) parameterisation suggests different formulation for each of the stability conditions. Furthermore, it includes the effect of rotation (say the Ekman layer) for the neutral conditions.

WSI extracts the SL scales needed for these parameterisations directly from WRF results. The Hanna (Hanna 1982) and Scire et al. (Scire et al. 2000) parameterizations are quite similar in their structures and mainly differ in the empirical curves used to calculate the wind velocity standard deviations. The Scire et al. (Scire et al. 2000) parameterisation used in WSI uses the SL scales extracted from the WRF simulation. To complete the turbulence parameterisation for SPRAYWEB, we need the Lagrangian time scales. Since the Scire et al. (Scire et al. 2000) parameterisation does not provide these quantities, being designed for Gaussian models, we take into account those given by the Hanna (Hanna 1982) parameterisations, also with the wind velocity standard deviation prescribed by Scire et al. (Scire et al. 2000).

The FFT-07 experiment

In September 2007, experimental release trials called "FUsing Sensor Information from Observing Networks (FUSION) Field Trial -2007" were performed at Dugway Proving Ground in Utah, USA (Storwald 2007; Platt et al. 2008). This short-range experiment (about 500 m) was meant to compare Source Term Estimation (STE) algorithms. It is also meant to use the collected information to point out the strength and weakness of different parameterisation (Singh and Sharan 2013).

In this work, we consider among the other three experiments characterised by different stability conditions, which are stable for Trial 07, unstable for Trial 45 and neutral for Trial 46, on the basis of the Obukhov length L whose values are 40, – 3 and 149 respectively. In all trials, the emission is continuous from a single source. The source height is 2 m, and its diameter is 3 mm. In the FFT-07 experiment, other trials were performed, but not all were available. Out of the total 80 trials, only 52 trials are conducted for continuous releases in which 21 trials correspond to single releases. Out of these 21 trials of single releases, data was available only for 10 trials. Unfortunately, we got only 7 trials. Accordingly, out of 7 trials of a single release in the FFT-07 diffusion experiment, 4 trials correspond to stable conditions, two trials to neutral conditions and only one to unstable conditions. Thus, we prefer to compare the same number of trials for each stability condition. In addition, we remark that the number of measurement stations in a single trial is 100, which guarantees sufficient statistics for analysis. It is also worth mentioning that we are interested in simulating plume and not puff at least in this work.

Observations were taken by a set of 100 digital PID (Photo-Ionisation Detector) samplers, arranged in a rectangular staggered grid/array of area 475m × 450m in 10 rows and 10 columns as shown in Fig. 1.

Sampler's height is the same as the one of the source. and the probe's grid was set to -25° from the North direction in order to take advantage of the prevailing wind flow (Pandey and Sharan 2018). PIDs were set in the flattest, most uniform and most homogeneous terrain in order to reduce the effect of the ground level mechanical turbulence. For each receptor, we have a series of data lasting about 10 min and measured at 50 Hz frequency, so we calculate the mean and variance from these series.

Results

Plot analysis

In Figs. 2–7, the scatter and qq-plots are shown for mean and standard deviation concentration and the two parameterisations. The same plots for the concentration intensity (the ratio between standard deviation and mean) are also reported. Comparing Fig. 2 with Fig. 3, the performances of the two parameterisations can be analysed. It can be observed that the scatter plots are different in the two cases. Those obtained using the Scire et al. (Scire

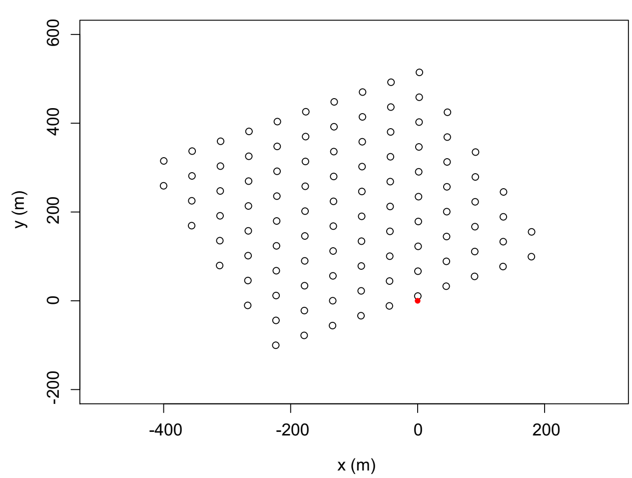

Fig. 1 Experimental set-up. The open circles indicate the probe positions and the red dot the source position. The x-axis is directed from West to East, and the y-axis is directed from South to North

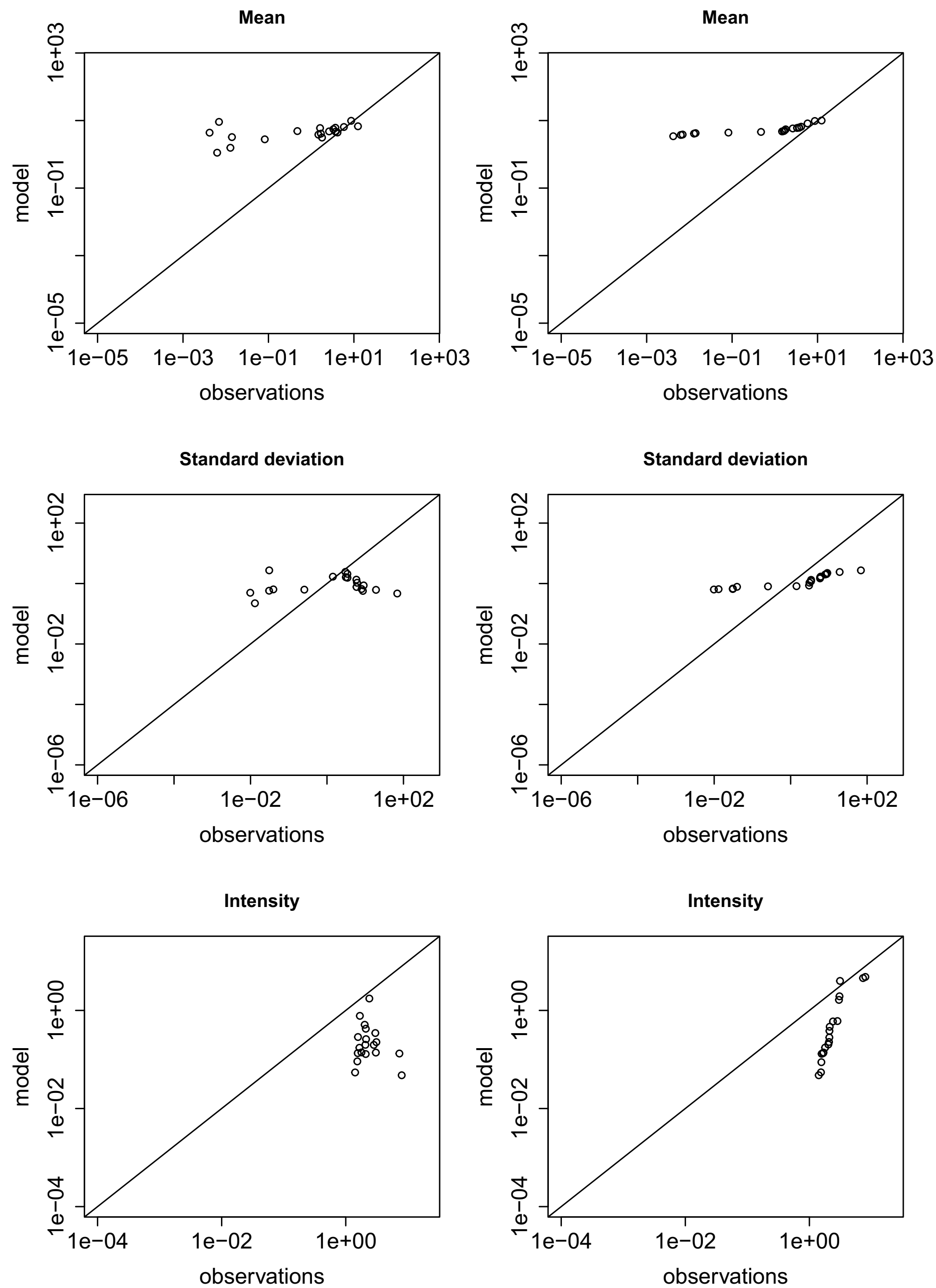

Fig. 2 Scatter-plots (top) and qq-plots (bottom) for Trial 7 (stable conditions) (g/m^3), for the Hanna (Hanna 1982) parameterisation

et al. 2000) parameterisation shows a larger scatter of the point around the line indicating "perfect agreement", both for mean and standard deviation concentration. The scatter plots also indicate that the results obtained using the Hanna (Hanna 1982) parameterisation vary in a smaller range with respect to those obtained with the Scire et al. (Scire et al. 2000) parameterisation. However, the qq-plot shows similar behaviour for the two parameterisations meaning that the distribution of the values (both mean and standard deviation) does not change in the two cases. In Figs. 4 and 5, the results obtained with the two parameterisations in the case of the Trial 45 can be observed. The results are similar in the two cases except for an underestimation of the concentration standard deviation and concentration intensity when the Scire et al. (Scire et al. 2000) parameterisation is taken into account. The model seems to perform better in neutral conditions (Trial 46). As can be observed in Figs. 6 and 7 both for mean and standard deviation concentration, the number of point in the plots is larger than for the cases of Trial

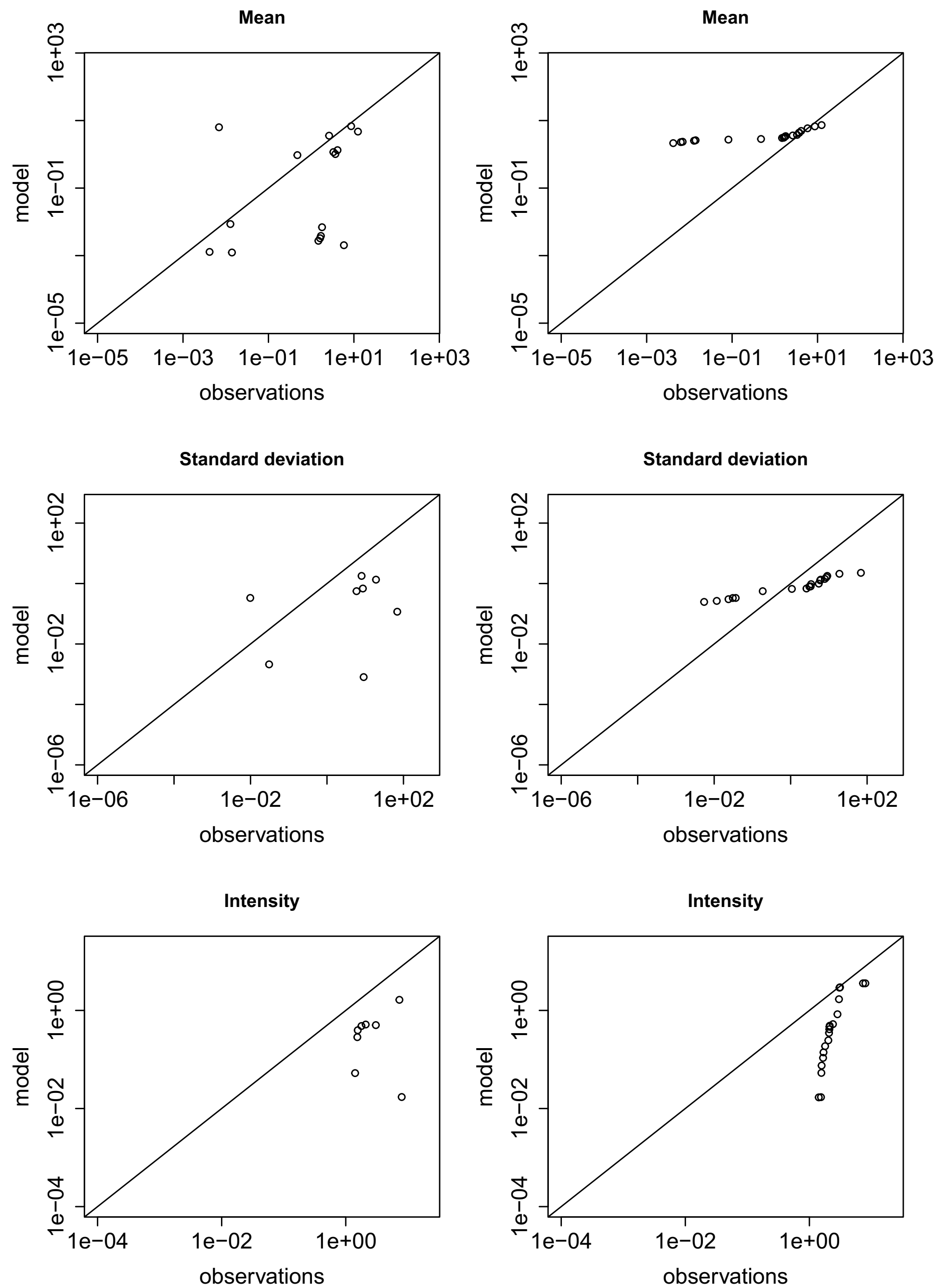

Fig. 3 Scatter-plots (left) and qq-plots (right) for Trial 7 (stable conditions) (g/m^3), for the Scire et al. (Scire et al. 2000) parameterisation

07 and Trial 45, which indicates less zeros in the calculated values. Highest values of the mean concentrations are better reproduced. The Scire et al. (Scire et al. 2000) parameterisation underestimates the concentration standard deviation's highest values.

Statistical analysis

For the statistical analysis, we considered the metrics suggested by Chang and Hanna (2004): mean value, Fractional Bias (FB), Normalised Mean Square Error (NMSE), factor of two (FAC2) and factor of five (FAC5).

The results of the statistical analysis in terms of the indexes are shown in Table 1 for the Trial 07, in Table 2 for the Trial 45 and in Table 3 for the Trial 46 respectively. The tables show the values of the indexes both for mean and standard deviation concentration and for the two parameterisations.

Concerning the Trial 07 (Table 1), both the parameterisations overestimate the observed mean concentrations but

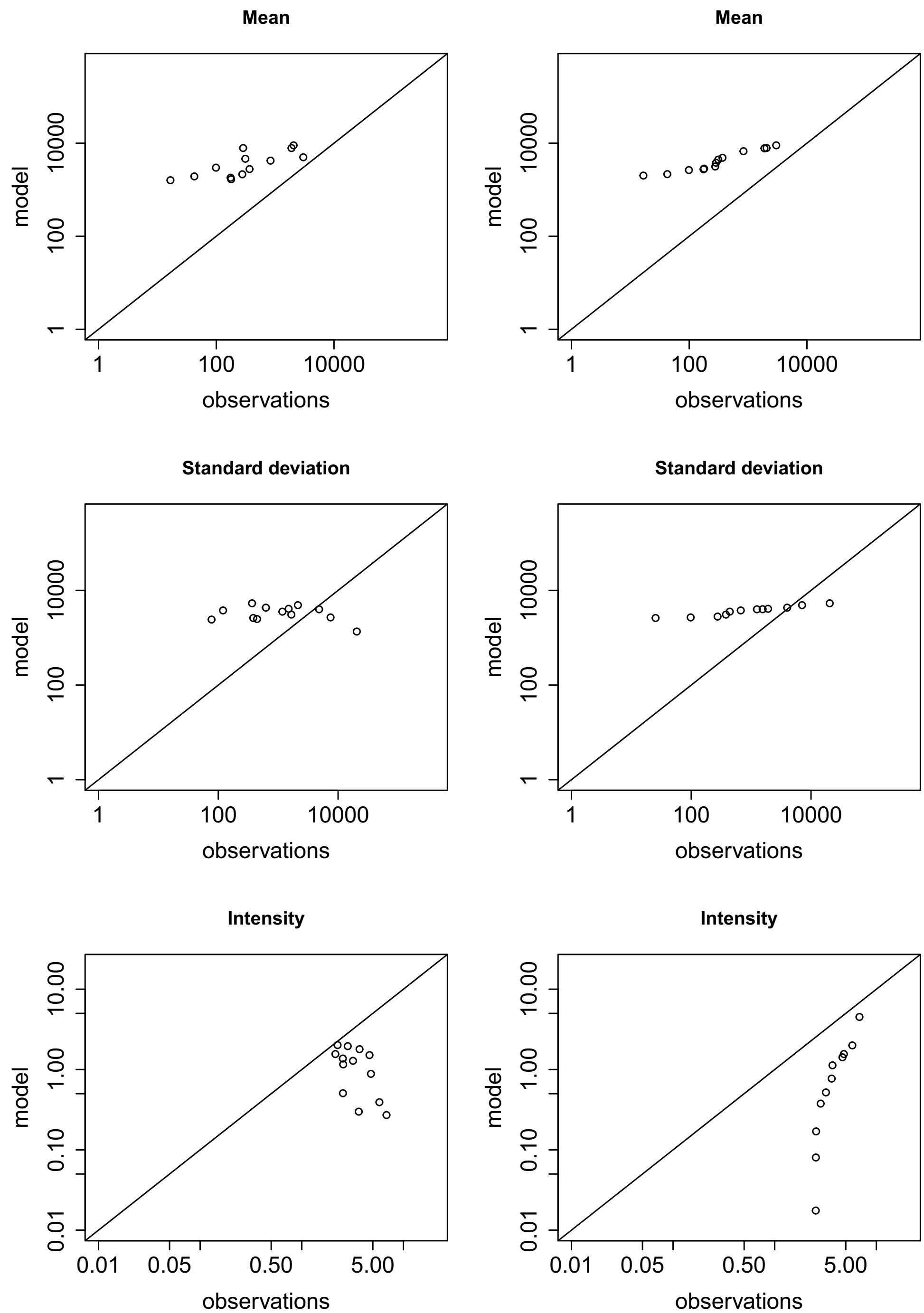

Fig. 4 Scatter-plots (left) and qq-plots (right) for Trial 45 (unstable conditions) (g/m^3), for the Hanna (Hanna 1982) parameterisation

the Scire et al. parameterisation to a lesser extent. On the contrary, the Hanna parameterisation better performs as NMSE, FA2 and FA5. As far as the concentration standard deviations are concerned, both the parameterisations underestimate the observations, but the Scire et al. parameterisation shows a much larger NMSE and very low FA2 and FA5. This indicates an underestimation of the measurements according to the value of FB and NMSE. This trial refers to stable conditions which are the most difficult to simulate. Looking at the parameterisation, it can be observed that the one suggested by Scire et al. (Scire et al. 2000) does not distinguish between neutral and stable conditions which instead can influence the dispersion in different ways. This limit can be the reason for such an unsatisfactory result.

Looking at Table 2, it can be observed that the performance of the Scire et al. (Scire et al. 2000) parameterisation is better than that of the Hanna (Hanna 1982) parameterisation for all indexes of the mean concentration. On the contrary, the concentration standard deviation seems to

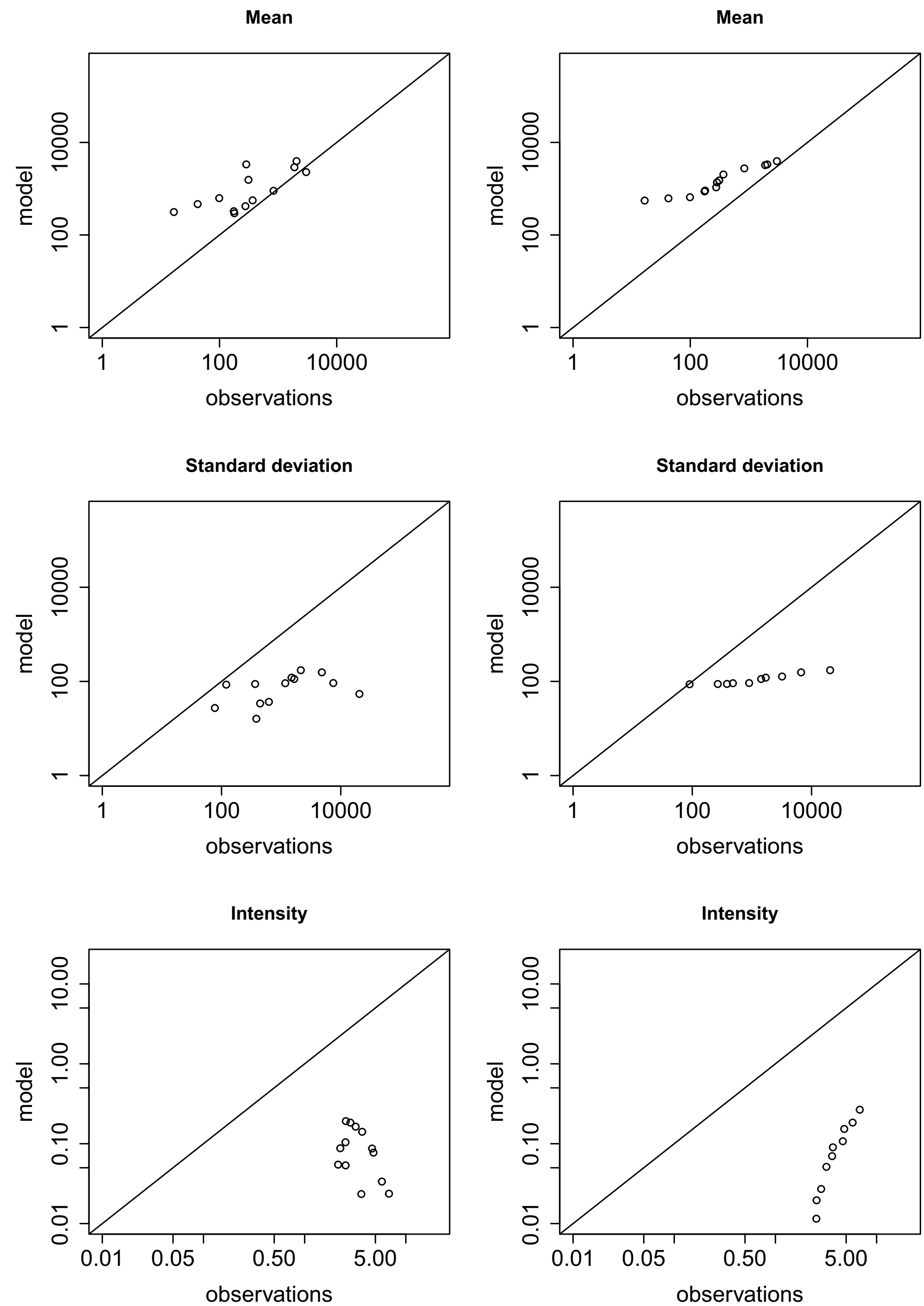

Fig. 5 Scatter-plots (left) and qq-plots (right) for Trial 45 (unstable conditions) (g/m^3), for the Scire et al. (Scire et al. 2000) parameterisation

be better reproduced by the Hanna parameterisation, which overestimates whereas the Scire et al. (Scire et al. 2000) parameterisation underestimates.

Considering the results of the statistical analysis of the results obtained in the Trial 45 (Table 3), it can be observed that, for the mean concentration, the performance of the two parameterisations are very similar except for FB which shows underestimation in the case of Hanna (Hanna 1982) parameterisation and overestimation in the case of Scire et al. (Scire et al. 2000) parameterisation. Also, the indexes relating to the concentration standard deviation are similar, but the Hanna parameterisation gives a lower NMSE and worse values for FA2 and FA5.

Generally speaking, it can be observed that the values of NMSE for the concentration standard deviation are very height, while the values of FB are lower. This demonstrates that the NMSE values at extreme heights are due to some single point, whereas the predicted mean values are closer to the observed ones.

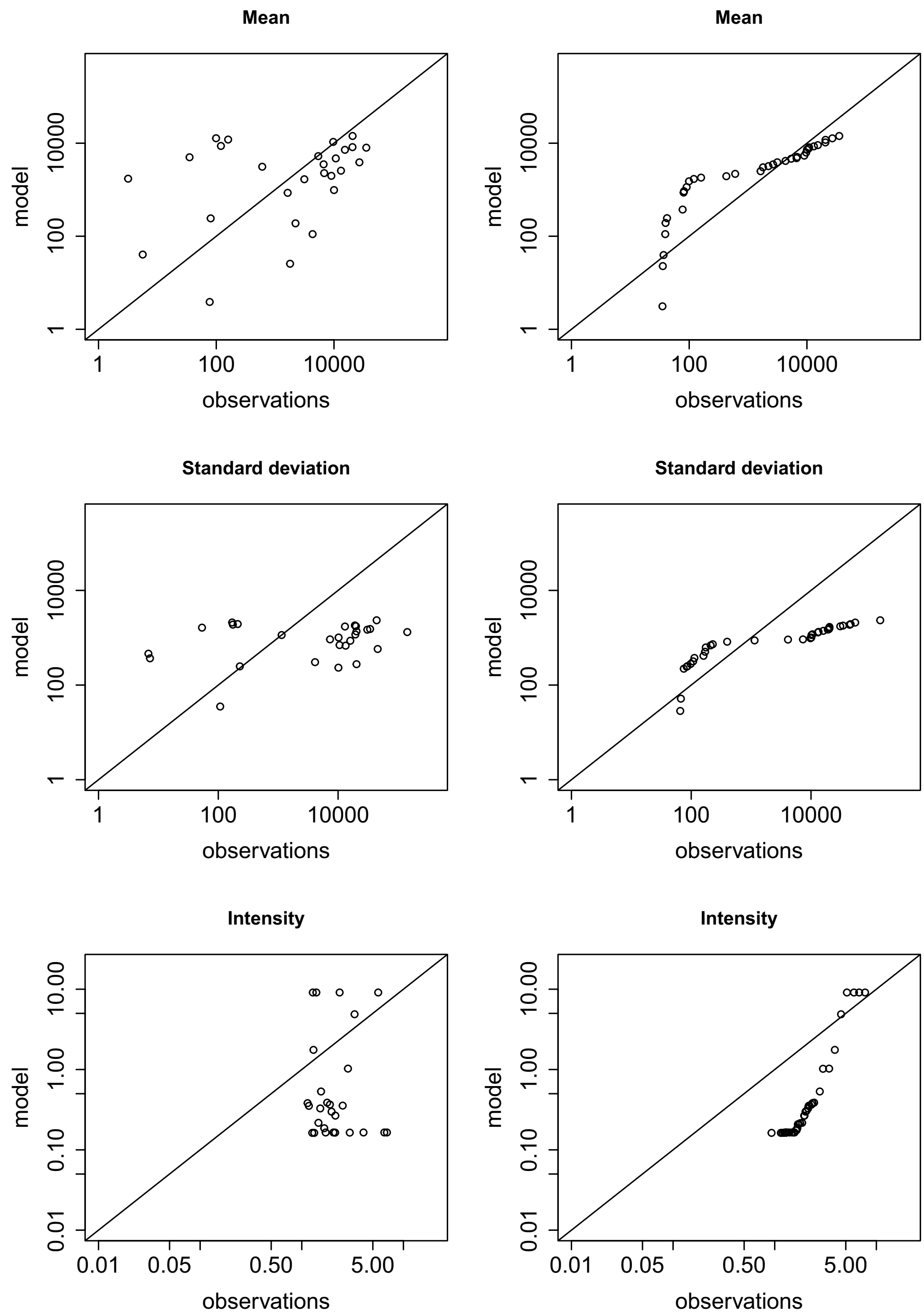

Fig. 6 Scatter-plots (left) and qq-plots (right) for Trial 46 (neutral conditions) (g/m^3), for the Hanna (Hanna 1982) parameterisation

Discussion and conclusions

In stable conditions, the horizontal velocity standard deviation in the Hanna (Hanna 1982) parameterisation does not depend on the Obukhov length, L, while in Scire et al. (Scire et al. 2000), it slightly increases for a higher value of L. As observed in "Plot analysis", the calculated mean and standard deviation concentrations vary in a wider range with the Scire et al. parameterisation with respect to those obtained using the Hanna (Hanna 1982) parameterisation which is due to the larger horizontal standard deviation. In fact, $L = 40$ for the Trial 7. However, the overall results obtained using the Hanna parameterisation show a better performance (except for FB).

On the contrary, in unstable conditions, the horizontal velocity standard deviation prescribed by the Hanna (Hanna 1982) parameterisation increases with L and remains unchanged in the case of Scire et al. (Scire et al. 2000). Thus, in both cases, the two parameterisations

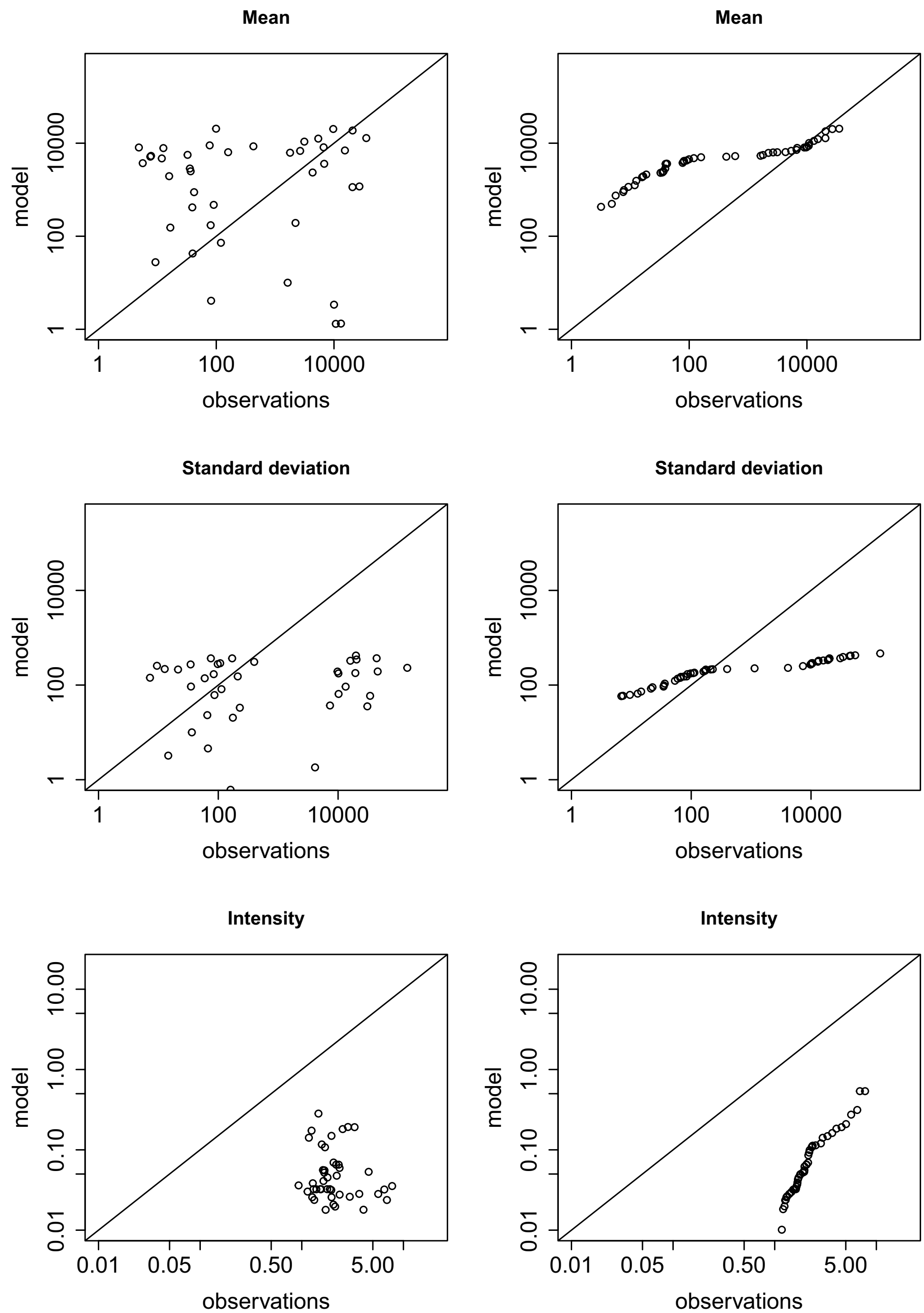

Fig. 7 Scatter-plots (left) and qq-plots (right) for Trial 46 (neutral conditions) (g/m^3), for the Scire et al. (Scire et al. 2000) parameterisation

Table 1 Statistical indexes for the Trial 07 (stable conditions)

Model	FB	NMSE	FA2	FA5	FB	NMSE	FA2	FA5
	Mean concentration				Standard deviation			
Hanna	− 1.0	5.8	47.4	63.2	1.3	89.8	21.1	36.8
Scire et al	− 0.5	7.7	21.1	47.4	1.5	173.1	0.0	9.1

differ the larger L is. As a matter of fact, being the values of L in the Trial 45 are very small (− 3), the two parameterisations do not differ too much.

Concerning the vertical standard deviation in the stable case, the two parameterisations show a similar profile which does not change with L.

Table 2 Statistical indexes for the Trial 45 (unstable conditions)

Model	FB	NMSE	FA2	FA5	FB	NMSE	FA2	FA5
	Mean concentration				Standard deviation			
Hanna	−1.6	35.7	7.7	23.1	−0.7	17.6	15.4	46.2
Scire et al	−1.0	11.3	61.5	69.2	1.8	550.4	7.7	23.1

Table 3 Statistical indexes for the Trial 46 (neutral conditions)

Model	FB	NMSE	FA2	FA5	FB	NMSE	FA2	FA5
	Mean concentration				Standard deviation			
Hanna	0.4	7.6	12.8	27.7	1.8	149.1	4.3	6.4
Scire et al	−0.2	6.0	12.8	31.9	1.9	507.0	8.5	29.8

In unstable condition, the two parameterisations show different values in the surface layer depending on the L value. For lower values of L, they show a similar profile, while for higher values of L, the Hanna (Hanna 1982) parameterisation got values about 5 times those given by the Scire et al. (Scire et al. 2000) parameterisation. Looking at the results of the statistical analysis in the table (Hinze 1959), Scire et al. (Scire et al. 2000) parameterisation seems to provide better results as far as the mean concentration is considered, while for the standard deviation concentration, the Hanna parameterisation gives more accurate results.

Concerning the neutral case Trial 46, the results obtained with the two parameterisations, that obviously do not depend on L, look very similar for the mean values, but better in the case of Scire et al. parameterisation as far as the standard deviation concentration is taken into account.

Generally speaking, both parameterisations provide results that are still not completely satisfactory. Some differences in the performances of the two parameterisations come out from this analysis because of the Obukhov length, L, which seems to play a role both in the simulation of the mean and the standard deviation concentrations. However, more effort must be done to improve the turbulence parameterisations as, for example, the turbulent kinetic energy or higher order moments of the velocity fluctuation probability density function. As far as we know, there are no standard models to calculate the variance concentration runtime as in our model. Standard models only simulate the mean concentrations, and this is one of the novelty of this work. On the contrary, there are some new models developed for research purposes such as SPRAYWEB.

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Data availability I do not have the rights to distribute the data.

Declarations

Ethics approval Not applicable.

Consent to participate Not applicable.

Consent for publication Yes.

Conflict of interest The authors declare no competing interests.

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