19th International Conference on
Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes
3-6 June 2019, Bruges, Belgium

EVALUATION OF TURBULENCE PARAMETRIZATIONS FOR LAGRANGIAN DISPERSION MODELS

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Abstract: The new meteo-dispersive modelling system SMART is under development and preliminary tests have been conducted. The final purpose is to offer the simulation and forecast of the atmospheric pollutant dispersion due to possible accidental releases in any part of the Italian territory at any time, as an operational suite for emergency response covering all the country is not available. Here the focus is on ARAMIS, the boundary-layer and turbulence parametrization module created to interface the non-hydrostatic atmospheric model MOLOCH and the Lagrangian stochastic dispersion model SPRAY into the SMART system. Since the parametrization of turbulence has a key role for dispersion modelling, we assess the turbulence parameterizations implemented in ARAMIS to prepare the fields needed by SPRAY, by evaluating three options for the standard deviations of wind velocity.

Key words: *Modelling suites, turbulence parametrization, Lagrangian particle model.*

INTRODUCTION

A new modelling suite, SMART (Spray - Moloch Atmospheric Regional Tool) is under development with the final goal of making available a numerical tool to forecast the pollutant dispersion from possible accidental releases in the atmosphere, in any part of the Italian territory at any time. At the CNR-ISAC daily meteorological forecasts are issued over all Italy at a high resolution, 1250 m, by applying the MOLOCH model, in support of research on the atmospheric circulation and composition and in order to test and improve the meteorological model itself. MOLOCH model integrates the non- hydrostatic, fully compressible equations for the atmosphere. Given the availability of these high- resolution forecasts, we developed a new module, ARAMIS, interfacing MOLOCH and the Lagrangian particle dispersion model SPRAY, and tested it in some case studies in different sites of Italy.

Here, after a brief description of the ARAMIS (Atmospheric Regional Algorithm for Moloch Interfaced to Spray) code, the results from some preliminary SMART simulations are analysed, in order to assess the performance and suitability of the different turbulence parametrizations in different atmospheric conditions. We examine the sensitivity of the turbulence closure scheme of the meteorological model to the resolution, by considering two horizontal grid spacings in MOLOCH, the standard 1250 m and a finer one at 500 m. Strong and low wind regimes are considered, in order to evaluate the ability of the three wind-velocity standard deviation parametrizations to capture the variability of the atmospheric dynamics. The assessment is conducted based on data collected at an urban site in north Italy, Torino. The effect of the different parametrizations on the atmospheric tracer dispersion is investigated through SPRAY simulations of idealized cases in two different days.

BRIEF DESCRIPTION OF ARAMIS CODE

As first step, ARAMIS code processes a mapping of MOLOCH coordinate system in order to build the proper system needed by SPRAY for its simulation domain. MOLOCH and SPRAY models both employ terrain following vertical coordinates, but not exactly the same. In MOLOCH a hybrid terrain following coordinate, relaxing smoothly to horizontal surfaces away from the earth surface, is used, while SPRAY use a sigma-coordinate system requiring a constant top of the domain. The horizontal coordinates are different as well. SPRAY uses a regular grid in metres, MOLOCH uses the spherical distances from a reference point, and thus an irregular and strewn grid. Therefore, appropriate interpolations are applied. Then ARAMIS calculates the turbulence variables required by SPRAY and not specifically provided by MOLOCH, such as the wind velocity standard deviations, focus of this work, and the Lagrangian time scales.

We tested three different methods to compute the wind velocity standard deviations $\sigma_u, \sigma_v, \sigma_w$ needed by SPRAY dispersion model. The first is a *K*-closure (*K-TH*) and it is based on the eddy-viscosity concept, determining the turbulent Reynolds stresses as proportional to the mean-velocity gradients:

$$\sigma_u^2 = -2K_{mx}\frac{\partial \overline{u}}{\partial x} + \frac{2}{3}E\ ,\ \sigma_v^2 = -2K_{my}\frac{\partial \overline{v}}{\partial y} + \frac{2}{3}E\ ,\ \sigma_z^2 = -2K_{mz}\frac{\partial \overline{w}}{\partial z} + \frac{2}{3}E \qquad (1)$$

where the K_{mi} are the diffusion coefficients and *E* is the turbulence kinetic energy.

As explained by Rodi (1980), the term $(2/3)E$ in addition to the classical formulation of the eddy-viscosity is necessary to make the expression applicable to the normal stresses. When considering only the first part with the velocity gradients, their sum would be zero because of the continuity equation. Thus, the additional term assures the normal stresses to be positive quantities and their sum to be equal to *2E*, as by definition of the turbulent kinetic energy:

$$E = \frac{1}{2}\left(\sigma_u^2 + \sigma_v^2 + \sigma_w^2\right) \qquad (2)$$

The second (*MY82*) is adopted from Mellor-Yamada (1982) closure, largely used in meteorological models, determining the wind velocity standard deviations through a direct proportionality to the turbulent kinetic energy *E*:

$$\sigma_u^2 = \left(\frac{1-\gamma_1}{2}\right)q^2,\ \ \sigma_v^2 = \sigma_u^2,\ \ \sigma_w^2 = \gamma_1 q^2 \qquad (3)$$

where $q^2 = 2E$ and γ_1 is a constant which empirical value is given as 0.22.

The third one (*SH82*) was formulated by Hanna (1982) and is based on classical boundary-layer theory and surface-layer parameters, and distinguish different expressions for the variances depending on the atmospheric stratification conditions, as:

in the unstable case: $\sigma_u = \sigma_v = u_*\left(12 + \frac{1}{2}\frac{z_i}{|L|}\right)^{1/3}$; $\sigma_w = f\left(w_*, \frac{z}{z_i}, \frac{L}{z}\right)$ (depending on $\frac{z}{z_i}$) (4)

in the stable case: $\sigma_u = 2u_*\left(1 - \frac{z}{h_e}\right)$, $\quad \sigma_w = \sigma_v = 1.3u_*\left(1 - \frac{z}{h_e}\right)$ (5)

in the neutral case: $\sigma_u = 2u_* \exp\left(-\frac{3fz}{u_*}\right), \quad \sigma_w = \sigma_v = 1.3u_* \exp\left(-\frac{2fz}{u_*}\right)$ (6)

The interest here lies in assessing the characteristics and performances of the alternative parameterisations, established from different approaches. In particular, the comparison between the formulations derived by the K-theory and the Mellor-Yamada closure allows investigating the contribution of the velocity gradients that might be critical quantities in complex topography when using atmospheric models, which provide variables that are grid-spacing dependent.

CONFIGURATION OF THE SIMULATIONS

In Trini Castelli et al. (2019) we conducted a series of MOLOCH simulations for 18 different days in 2007, for which we had observed data available, for assessing the capability of the model in evaluating the turbulent kinetic energy (TKE). The site of interest is located in the CNR research area in the southern outskirts of Torino city (north-west Italy), where an experimental campaign was conducted in 2007-2008 (Trini Castelli et al., 2014). Data from three sonic anemometers at different heights are available.

Here we choose two days, February the 13^{th} characterized by strong wind, and October the 1^{st}, whose main feature was the low wind. First we compare the simulated and measured TKE, as it is the main input for calculating the velocity standard deviations in *MY82* and *K-TH* parameterizations. Then we estimate the agreement between observations and simulations for the velocity standard deviations, by considering all three ARAMIS options. Finally, we specifically analyse the single terms of the *K-TH* formulation, since the velocity gradients included in it are sensitive to the numerical discretization given by the grid spacing.

SPRAY simulations were performed for both days with all three turbulence formulations. We consider a point source, a 20-m high stack with a diameter of 0.6 m, emitting 10^9 µg of NO_x per hour. The emission is characterised by a vertical exit speed of 1.2 ms^{-1} and by a temperature of 180 °C. For the SPRAY concentration grid we choose the same resolution as in MOLOCH. We compare the resulting concentration fields in a qualitative way, since no observed data are available.

RESULTS, DISCUSSION AND CONCLUSIONS

In **Figure 1** the comparison between the TKE measured at 25 m, in the inertial sublayer, and the simulated TKE, representative of the first atmospheric layer above the surface, is shown together with the derived vertical standard deviation, for both the strong and low wind cases. MOLOCH exhibits good performance in detecting the location of the TKE peaks for both the resolutions in the strong wind case. Nevertheless, the higher resolution, 500 m, allows MOLOCH to better match the observed data, while with the lower resolution, 1250 m, the data is underestimated. For the low wind case, the single peak is very well captured by MOLOCH and the agreement between predictions and observations is good with both resolutions. Given the better agreement obtained with the 500 m resolution for the TKE, here the velocity standard deviations are plotted and analysed for this model configuration.

The comparison between the measured and simulated vertical standard deviation is good for both strong and low wind cases and for all parametrization options. More in detail, for the strong wind case we obtain higher values with the *K-TH* formulation, intermediate values with *MY82,* and smaller values with *SH82*. However, the differences are relatively small and all the three options are able to capture the peaks. For the low wind case, we notice a left shift of *SH82* parametrization with respect to the other two that are in phase (bottom-right panel of figure 1). *K-TH* option produces slightly higher values. We note that a lower threshold of 0.2 ms-1 is assigned to the vertical standard deviation in the numerical simulation. Similar considerations can be done for the horizontal standard deviations (not shown) for *MY82* and *SH82*. Instead, the *K-TH* scheme gives very fluctuating values, often beyond sensible threshold, here considered as 2.5 ms^{-1} for the maximum and 0.25 ms^{-1} for the minimum.

Given this result, in Figure 2 we analyse all single terms determining the horizontal standard deviation in the *K-TH* configuration. It can be seen that the diffusion coefficients *Kx* calculated by MOLOCH can take rather high values, in particular for strong wind speeds. In this case, when in correspondence the velocity gradients have absolute values around the unit, their product with the diffusion coefficients can take large and fluctuating values, possibly leading to non-sensible values of the related horizontal standard deviation. In MOLOCH the horizontal diffusion coefficient is calculated based on an *E-l* turbulence closure and using a mixing length proportional to the horizontal grid spacing. Thus, the horizontal diffusion has a numerical aspect that can overcome its physical meaning, as common in mesoscale atmospheric models. Using the diffusion coefficients for the velocity fluctuations, as in *K-TH* formulation, at this scale and in some conditions can be critical, so this issue needs further investigation.

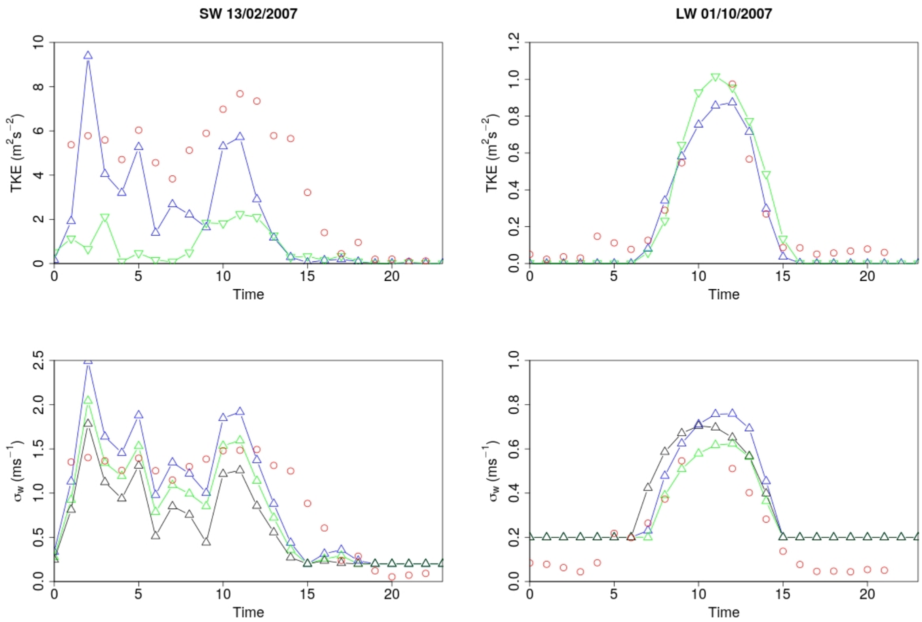

Figure 1. Left: strong-wind case 13/2. Right: low-wind case 1/10. Top: measured (red circles) and simulated TKE at 1250 m (green) and 500 m (blue) grid spacing. Bottom: vertical standard deviation from *MY82* (green), *K-TH* (blue) and *SH82* (black) formulations at 500 m grid spacing

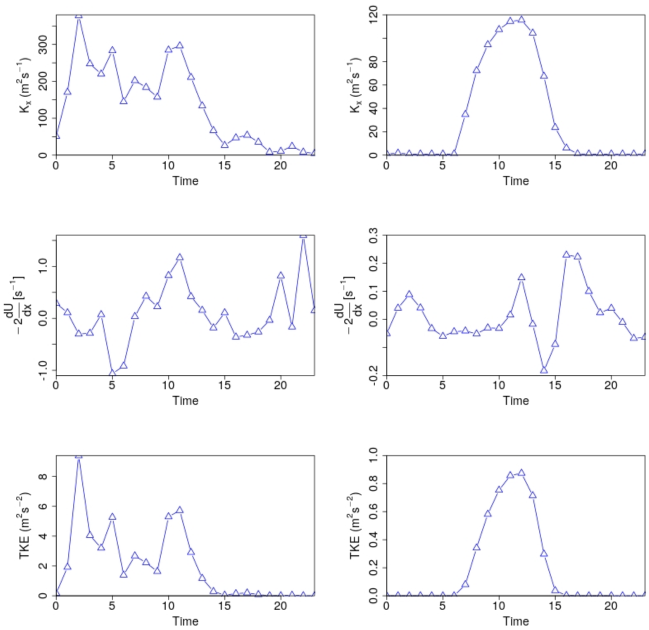

Figure 2. Plots of the different terms of *K-TH* formulation.
Left: strong wind on 13/2/2007; right: low wind on 1/10/2007

In Figure 3 the concentration field produced by SPRAY simulations are shown. Again we compare the three turbulence parametrization options. For the strong wind case, *MY82* and *SH82* parametrizations give very similar results, while the *K-TH* formulation shows lower concentration near the source and a slightly larger area of impact. The difference can be due to the larger diffusion characterizing the *K-TH* case, both in the vertical and horizontal. For the low-wind case, *MY82* and *K-TH* lead SPRAY to produce similar concentration fields, with slightly higher values for *MY82*, while with *SH82* the pattern is a bit different since the impact area far from the source is reduced with respect to the others. However, only one-day simulations have been considered here, thus these results are not necessarily indicative and cannot be generalized.

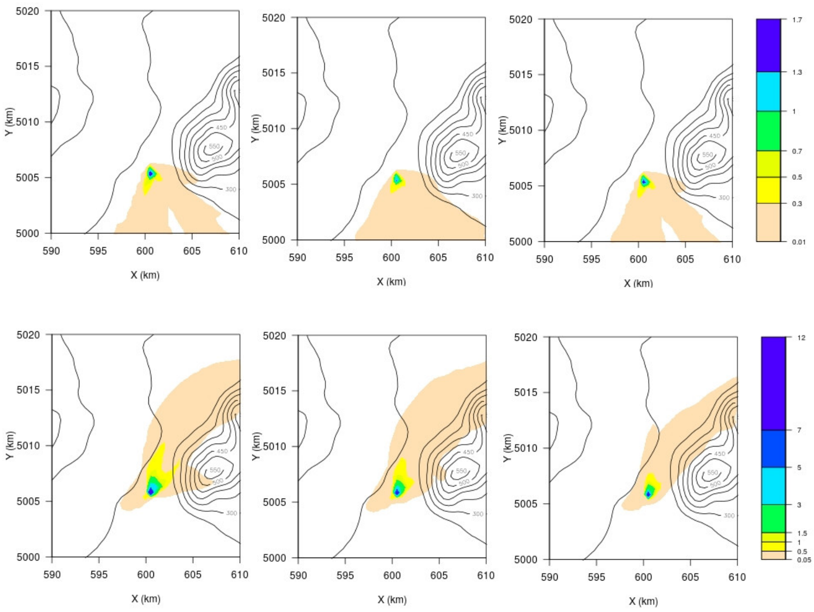

Figure 2. Concentration field of SPRAY simulations. Top: strong wind case on 13/2; bottom: low wind case on 1/10. Left: MY82 formulation; centre: *K-TH formulation;* right: *SH82* parametrization.

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