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# WRF PBL SCHEMES FOR TURBULENCE PARAMETERIZATIONS: REPRESENTING DISPERSION PROCESSES IN SUB-KILOMETER HORIZONTALLY NON-HOMOGENEOUS FLOWS

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**Abstract**: The simulation of dispersion processes over complex terrain is challenging as it directly relies on the availability of accurate meteorological fields, particularly in terms of wind velocity and direction, atmospheric stability, including thermal structure and turbulence. Over complex terrain, these fields are typically strongly non-homogeneous and an inaccurate estimate of their distribution has a direct impact on the fidelity of pollutants' dispersion prediction. To properly describe meteorological fields over complex terrain, mesoscale models may be run with a sub-kilometer horizontal resolution, to allow for an accurate description of the topography. However, high-resolution simulations may not satisfy the underlying assumptions supporting the design of mesoscale parameterizations. Specifically, the assumption of horizontal homogeneity for mixing schemes is violated as grid spacing decreases and this inconsistency can generate issues in the results obtained with this standard approach. In this analysis, we present preliminary tests run with the WRF model (Skamarock et al., 2008) and the SPRAYWEB Lagrangian dispersion model (Tinarelli et al. 2000; Alessandrini and Ferrero 2009), assessing the ability of the WRF Nakanishi and Niino (2004) 1D PBL scheme in providing information to use in the turbulence parameterization for the dispersion model. For the evaluation of the PBL scheme, near-ground concentration observations are considered from the Bolzano Tracer EXperiment (BTEX – February 2017).

***Key words:*** *complex terrain, turbulence parameterizations, PBL scheme, dispersion modeling*.

## INTRODUCTION

Different modeling chains for the simulation of a local-scale tracer release from an incinerator plant are tested, over complex terrain. Ground concentrations from the BTEX field campaign are used to evaluate the performance of the models put to test. During the 2017 campaign, two tracer releases from the chimney of the Bolzano incinerator (Western Italian Alps) were performed, one in the early morning and one in the early afternoon, and samples of ground concentrations were collected (79 samples). Meteorological simulations are run with the WRF model to reconstruct the flow field with a sub-kilometer grid (300 m) and with observational nudging of upper-air and surface meteorological observations. The meteorological simulation has been optimized by modifying the snow cover initialization of the WRF model to improve the prediction of valley winds in the afternoon. These optimized meteorological fields are fed into the WSI/SPRAYWEB Lagrangian particle model. The SPRAYWEB model is run with different parameterizations implemented in the WRF-SPRAYWEB Interface (WSI) for the calculation of the wind velocity standard deviations and of the Lagrangian time scales. An additional test is also run by substituting the closure constants of the WRF PBL scheme with a set of constants obtained for complex terrain applications. A statistical analysis of the results from all the models is conducted to evaluate the simulation performance against concentration measurements.

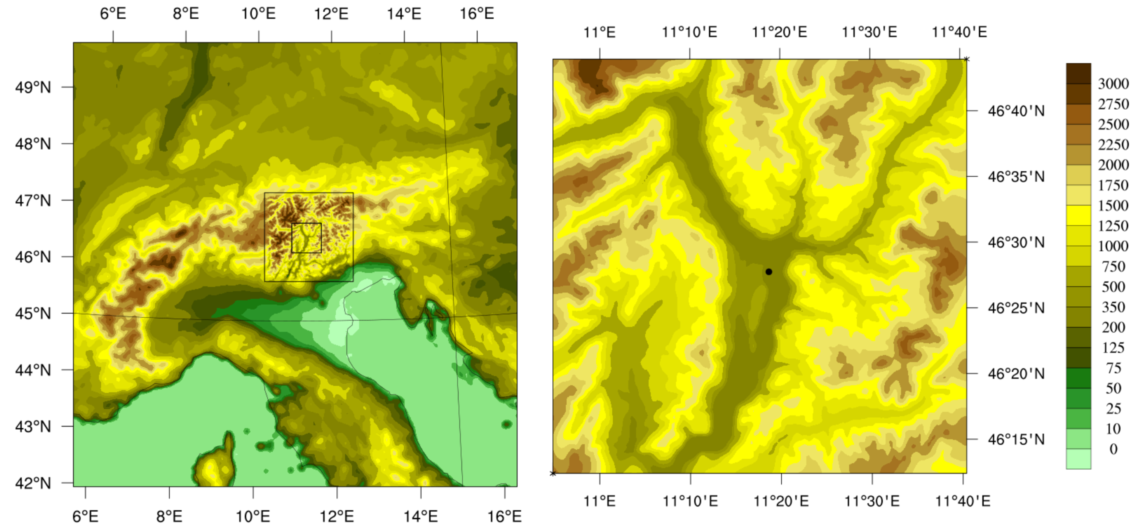


**Figure 1.** WRF nested domains from Northern Italy to the Bolzano basin with their elevation contours. The dot in the right panel indicates the location of the incinerator plant.

## METEOROLOGICAL SIMULATIONS

Simulations are run over the Bolzano basin on 14 February 2017, when the BTEX tracer releases were performed, in order to reconstruct the meteorological field and the concentration field of the tracer. The WRF simulation is run at a sub-kilometer resolution to provide reliable meteorological fields for the dispersion simulations. WRF v.3.8.1 is run with 3 two-way nested domains (Figure 1) and hourly observational nudging in the innermost domain. The external domain runs on a 4.5-km horizontal grid, and a 300-m resolution is reached in the innermost domain. Such a fine grid in the external domain is appropriate as the boundary and initial conditions for the simulations come from 6-hourly ECMWF HRES Operational Data, with 9-km resolution. The vertical grid of the simulation is composed of 62 vertical levels distributed so that the resolution is finer closer to the ground: 10 levels lie in the first 300 meters from the ground, evenly spaced each 30 m, and other 14 levels lie between 300 m and 1 km. The simulation covers the release day of BTEX. Static data for the two external domains come from default WRF data sets, with a resolution of 30" for both the topography and the land use. For the innermost domain, 1" topographic data and 3" land use cover data (Corine Land Cover data reclassified to the IGBP Land Cover Type Classification) are provided. The 1.5-order Nakanishi and Niino (2004) scheme for the Planet Boundary Layer parameterization is used. The effects of shading and slope angle in complex terrain are taken into account and topographic wind correction is applied for the two external domains. The simulation runs with hourly observational nudging of all the available meteorological observations, including: (i) wind speed and direction, temperature and relative humidity from 15 weather stations; (ii) 2 vertical wind profiles from a SODAR instrumentation on the incinerator roof, and from a LIDAR at the exit of the Isarco Valley; and (iii) 1 vertical temperature profile from the thermal profiler located South of the city of Bolzano. Preliminary results from the WRF simulation showed that the model generated a strong drainage wind in the lowest layers, which flew from the upper Adige Valley toward the Bolzano basin, in the early afternoon. This drainage flow was not recorded by any of the assimilated weather station observations, which indeed show very low wind intensities. The presence of such a strong flow could be very problematic for the dispersion simulations: indeed, given its height, direction and timing, this flow reached the Bolzano basin and hit the incinerator plant, clearly influencing the plume dispersion trajectory. For this reason, a detailed analysis of the causes generating this phenomenon was carried out and the cause of the development of this local phenomenon was found to reside in an erroneous initialization of the snow cover. As no snow was present over the study area during the day of the release, the initialization of the snow cover in the WRF model was modified, intervening by completely removing the presence of the snow. With this intervention, the upper part of the Adige Valley is characterized by lower wind speeds and the wind flow is hardly organized in prevalent directions. The overall results of the meteorological simulation are therefore satisfactory and represent a rather reliable input for the dispersion models.

## DISPERSION SIMULATIONS

In order to reproduce the dispersion pattern of the released tracer, dispersion simulations are run with the SPRAYWEB model. Dispersion simulations start at 7 LST, when the first release from the chimney was performed, and end at 18 LST, 5 hours after the second release. In both the dispersion models the incinerator chimney is simulated as a point source, emitting at 60 m a.g.l a constant concentration of tracer throughout the duration of each release. SPRAYWEB is fed with the output of the WRF simulation, by means of the WSI. Being a Lagrangian model, SPRAYWEB does not require to fix neither vertical nor horizontal grid resolutions. Nevertheless, ground concentrations are returned on a grid with 300-m horizontal and 20-m vertical resolutions. The SPRAYWEB simulation runs with a varying time step which is internally calculated by the model, on the basis of the Lagrangian time scale values. Minimum time step is set to 2 s and 100 particles are released at every time step. Static data are directly read from WRF, and have therefore the same characteristics as in the meteorological simulation. The WSI is run with 3 different parameterizations for the turbulence characterization and 3 simulations with SPRAYWEB are therefore performed. Simulation $SPW_H$ runs with the Hanna (1982) parameterization, calculationg wind standard deviations and Lagrangian timescales from surface layer parameters. Simulation $SPW_{TKE}$ and simulation $SPW_{TKEmod}$ use the turbulent kinetic energy TKE and the vertical dispersion coefficient to obtain the wind standard deviations and the Lagrangian timescales (Mellor and Yamada 1982, Ferrero et al. 2003). $SPW_{TKEmod}$ differs from $SPW_{TKE}$ because different closure constants ($A_1$, $B_1$, $A_2$, $B_2$) are used both in the interface parameterization and in the WRF simulation. This new set of closure constants was obtained by Trini Castelli et al. (2001) for applications over complex terrain and should be therefore more suitable for the present case study.

## RESULTS

In order to evaluate the performance of the different models and parameterizations, different statistical indexes have been calculated, including: the correlation (R), the fractional bias (FB), the normalized mean square error (NMSE) and the factor 2 (Chang and Hanna 2004). Values of these indexes are reported in Table 1.

**Table 1.** Statistical indexes calculated for each air quality dispersion simulation. Bold font indicates the most performing value for each index.

| Simulation | meanOBS (pptv) | meanMOD (pptv) | R | FB | NMSE | f2 |
|---|---|---|---|---|---|---|
| $SPW_H$ | 900 | **893** | **0.8** | **-0.01** | **1.3** | **0.4** |
| $SPW_{TKE}$ | 900 | 441 | 0.7 | -0.7 | 5.0 | 0.3 |
| $SPW_{TKEmod}$ | 900 | 888 | **0.8** | **-0.01** | 2.2 | **0.4** |

The Lagrangian model SPRAYWEB performs differently with each turbulence parameterizations tested. The first two SPRAYWEB simulations share the exact same wind field and the differences identified in their performance can therefore be attributed to the dispersion only. Simulations $SPW_H$ performs very well against observations accurately predicting the mean value; the R value is very high and the |FB| and NMSE values are very low. With such a good performance, this simulation fulfills the acceptance criteria by Chang and Hanna (2012). $SPW_{TKE}$ simulation was expected to have a good performance, as it relies on the TKE values which are calculated with a prognostic equation in the PBL scheme (and should therefore carry more reliable physical information with respect to the SL scales). On the contrary, results from $SPW_{TKE}$, running with the parameterization decomposing the TKE on the three directions, show many deficiencies. First of all, the model presents the worst values for the mean and the fractional bias, underestimating the mean value of 50%. The NMSE also is high and f2 is low. It is therefore likely that the values of TKE and $k_M$ produced by the PBL scheme are inaccurate. Under this hypothesis, the test of $SPW_{TKEmod}$ was carried out. As the Nakanishi and Niino (2004) PBL scheme applied in WRF relies on turbulence closure constants which have been calibrated for flat terrain, these closure constants were substituted both in the WRF PBL scheme and in the WSI with values obtained for applications over complex terrain (Trini Castelli et al. 2001). Different performances of $SPW_{TKEmod}$ with respect to the other SPW simulations can be produced by both the slight modification of the mean flow and of the TKE and $k_M$ values (coming from the modified WRF simulation) and the modification of the closure constants in the turbulence parameterization. With the new closure constants, the SPRAYWEB simulation greatly improves its performance. Statistical indexes calculated for the $SPW_{TKEmod}$ simulation are comparable with $SPW_H$ indexes except for the NMSE value. The modeled mean gets very close to the observed value and R, NMSE and FB experience relevant improvement with respect to the $SPW_{TKE}$ simulation. The comparison of $SPW_{TKEmod}$ with $SPW_{TKE}$ results to be particularly meaningful: the exact same PBL scheme can produce very different results depending on just the closure constants which are applied. It is likely that the modification of these constants has an effect on both the flow field and the TKE and $k_M$ values.

## FINAL REMARKS AND FUTURE WORK

Further analyses are needed to better undestand the preliminary results presented. Work is planned in order to: understand which meteorological simulation is the best one for the present case study; run the $SPW_H$ simulation with the updated meteorological field and evaluate its performance; compare modeled wind standard deviations with observations from the SODAR instrumentation installed over the incinerator roof. In addition, a new 3D PBL parameterization is under developement for the WRF model which will be particularly suitable for applications at a local scale and over complex terrain, as it introduces a calculation of 3D turbulent fluxes and the divergence. This new 3D PBL scheme should greatly improve the results of the PBL scheme in terms of TKE and dispersion coefficient, leading to even better results in terms of dispersion simulation using the PBL information. Indeed, a 3D reconstruction of the dispersion coefficients would allow a more accurate calculation of the Lagrangian timescales on the the three directions (Ferrero et al. 2003). The formulation of the 3D PBL scheme is based on the turbulence model developed by Mellor and Yamada (1982). The implementation in the Weather Research and Forecasting (WRF) model is proceeding in steps from a pure algebraic model that diagnoses the turbulent kinetic energy (TKE) equation to a higher level model that predicts the TKE. During each step, we compare results from the 3D PBL parameterization with both state-of-the-art 1D PBL and large eddy simulations (LES). At the actual stage of the development of the new scheme, it allows applications on idealized cases only, and tests are ongoing over idealized and schematic valley geometries. In the near future, the 3D PBL scheme will be also available for real cases and tests over the Bolzano Basin with data from the BTEX experiment are planned.

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