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COMPARISON OF DIFFERENT DISPERSION MODELLING APPROACHES IN COMPLEX TERRAIN

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Abstract: In the present study we focus on comparison and evaluation of results of different approaches for passive tracer dispersion modelling in complex terrain. Simulations with different meteorological and dispersion models are performed for selected episodes. Meteorological models included in the study are diagnostic mass-consistent wind field models and complete prognostic non-hydrostatic mesoscale model, while lagrange and euler approach are used for modelling the dispersion of polutants.

Key words: passive tracer, dispersion modelling, complex terrain, Austal, Calmet, Calpuff, WRF-Chem.

INTRODUCTION

Numerical air quality models present a primary tool for studying and forecasting air quality. Due to abundance and complexity of processes involved, their outputs can contain significant uncertainties. Dispersion of pollutants over areas with complex terrain is especially challenging to model due to strong local and meso-scale thermal and orographic forcings within the lower troposphere.

In the present study the area of interest is placed over the wider area of Ljubljana basin, a basin in the center of the country around the capital city of Slovenia. The basin with a bottom at 300 m a.s.l. is almost entirely surrounded by high mountains, reaching and exceeding 2000 m a.s.l. and only towards the SE the hills are lower. So the winds are often – especially during the cool air pool episodes in the basin – rather weak. In (the rather rare) occasions with stronger winds these are strongly orographically modified – with a lot of chanellings along the main axes of the basin and along its lateral valleys, with a lot of blockings, etc. So the reproduction of the reliable 3D wind filed is for this area a very challenging task.

The purpose of our study is to evaluate and compare results of simulations performed with different model types for a point source placed in the Ljubljana basin. Namely, models used represent different wind fields and turbulence dispersion representations, and use different dispersion modelling approaches – from modelling meteorological conditions with the complex meso-scale weather prediction model and modelling dispersion of pollutants with Eulerian approach, to modelling of wind field with only a simple diagnostic model and pollutant dispersion by Lagrangean approach.

MODELLING APPROACH

Three different modelling systems were used in our study and their results are compared for two different episodes. The first model is AUSTAL2000 (VDI, 2000) atmospheric dispersion model, developed in Germany under contract to the Federal Ministry for Environment, Nature Conservations and Nuclear Safety. It is the reference dispersion model, accepted as being in compliance with the requirements of Slovenian legislation demands for dispersion modelling in the smooth terrain, i.e. for emission sources in non-complex conditions (not over complex terrain, not at coastline, not for urban heat island etc.). The meteorological pre-processor in AUSTAL2000 model consists of diagnostic mass-consistent wind field model TALdia. The second modelling system consists of a diagnostic mass-consistent meteorological CALMET (Scire *et al.*, 2000a) model, and CALPUFF (Scire *et al.*, 2000a) air quality dispersion model, proposed by US EPA as a guideline model for regulatory applications involving situations where factors such as spatial variability in the meteorological fields, calm winds, fumigation, recirculation or stagnation and terrain or coastal effects may be important. Both diagnostic meteorological models (CALMET and TALdia) calculate wind fields diagnostically, using the variational approach to satisfy mass consistency and some measured wind data.

The third modelling system, WRF-Chem (Skamarock *et al.*, 2008; Peckham *et al.*, 2008), is a prognostic non-hydrostatic meteorological meso-scale model with complex parameterizations of different physical processes, turbulent kinetic energy prediction, radiation schemes, and fully online coupled chemistry and dispersion of pollutants.

| Experiment | Model | Other |
|------------|----------------|---------------------|
| А | Austal2000 | - |
| В | CALMET/CALPUFF | - |
| С | WRF-Chem | - |
| D | WRF_Chem | PBL parametrization |

Table 1. Experimental runs.

Configuration of models

All models were run in domain with 100x100 horizontal points and with 300 m horizontal resolution (Fig. 1). For the diagnostic wind field calculations in CALMET meteorological measurements at stations S1 and S3 (Fig. 1), and radiosounding measurements (Fig. 1) were used, while AUSTAL was run only with measurements at S1 station. For WRF model meteorological initial and boundary conditions were extracted from archived ECMWF meteorological analyses. WRF model was run in three one-way coupled domains (Fig. 2) with resolutions 5 km, 1 km, and 300 m, and with 45x45, 81x81 and 100x100 horizontal points, respectively.

Vertical atmosphere structure was in the two diagnostic meteorological models (Exp. A and B – compare Tab. 1) represented by 12 vertical levels from 0 to 2500 m altitude (Exp. A and B, Tab. 1). WRF model was set-up with 12 vertical levels identical to levels in diagnostic models, and with additional 27 levels extending up to 50 hPa. WRF model was configured without (Exp. C) and with (Exp. D) planetary boundary layer (PBL) parameterizations. Characteristics of point source were identical in all simulations, They are presented in Tab. 2. Dispersion of SO_2 , NO_x and PM10 was simulated in all experiments, but only results for SO_2 are presented.



Figure 1: Modelling domain, 100 x 100 points, with a) terrain height, b) area with dominant fraction of urban land cover category (indicating Ljubljana city), both in 300 m resolution. Shown are locations of three monitoring sites in the area, radiosounding location, and point source location.



Figure 2: Modelling domains representing the nesting strategy in WRF-Chem model. The innermost D3 domain coincides with modelling domain of CALMET/CALPUFF and AUSTAL2000 models, shown in Fig.1. Topography is shown in 5 km resolution, as represented in outer D1 domain.

Table 2. Point source characteristics.

| Latitude | Longitude | Stack height | Stack diameter | Velocity | Temperature | SO ₂ flow |
|-------------|------------|--------------|----------------|-----------------------|-------------|-------------------------|
| 46.05833 °N | 14.5495 °E | 100 m | 6 m | 6.4 ms^{-1} | 400.1 K | 240.3 kgh ⁻¹ |

Selected episodes

Two episodes, one winter (14. February 2008) and one summer episode (3. July 2008) were selected for simulations. Both episodes are characterized by anticyclonic meteorological situation, weak external dynamical forcings, and consequently relatively weak winds in the lower troposphere. Maximum measured ground level daily temperatures were between 0 °C and 3 °C in the winter case, and between 27 °C and 31 °C for summer episode. Radiosounding measurements in Ljubljana at 3 UTC showed subsidence temperature inversion between 900 m and 1200 m for winter day, related to high pressure

meteorological situation. Winds measured at 10 m height at station S1 (Fig.1) were slowly intensifying during the 15. February 2008, from 1 ms⁻¹ during the first night and forenoon, to 4 ms⁻¹ around the midnight 24 hours later. On the summer day the radiosounding at 3 UTC measured a night time temperature inversion between 250 m and 500 m, which disappeared by daytime air heating from surface and vertical mixing. Wind speeds measured at S1 station on the 3. July 2008 were up to $\sim 1 \text{ms}^{-1}$ until 10 UTC, and became stronger in the afternoon hours (maximum wind speed measured was 5.2 ms⁻¹ at 16 UTC).

Air quality measurements at S1 station showed rather low NOx and SO2 levels, while daily PM10 value was 29 μ gm⁻³ for 3. July and 96 μ gm⁻³ for 14. February, which is almost twice the daily threshold value (50 μ gm⁻³).

RESULTS AND DISCUSSION

Analysis of simulation results showed significant differences in pollutant concentration fields. For example, Fig. 3 compares fields of 1h daily maximum density values for SO₂ (in μ gm⁻³) on winter day, and Fig. 4 on summer day. On winter day for daily 1h SO₂ maximum field patterns are relatively similar among experiments (Fig. 3). The exception is Exp A, where there is no distinct maximum west of point source (as it appears in other experiments). On summer day field patterns for Exp B are inconsistent with other experiments; south western flow dominated in this experiment, while other simulations showed the prevalence of north eastern (Exp A, C) or northern (Exp D) flow. For both episodes pollutants are most dispersed in Exp A, while plume most maintains its directions and is the least dispersed in Exp B.



Figure 3: Comparison of ground level 1h daily maxima for experimental runs A-D (Tab. 1) performed for 15. February 2008. Please note that scale is figure dependant – legend maximum value (max) is shown in figure title.

The comparison of the maxima of daily 1h maximum fields (Fig.3 - 4 and Tab. 3) and the maxima of average 24h fields (Tab. 4) shows significant differences among experiments. Exp B is consistently related to the highest near ground air pollutant maxima, while in WRF-Chem simulations these maxima are at least for the factor of 0.73 lower for 1h daily maxima. For 24h averages maximum values in WRF-Chem experiments (Exp C, D) are even for factor of 0.24 to 0.1 lower than in Exp B, which is a consequence of stronger dispersion in WRF- Chem simulations, where simulated winds were stronger and more variable (see Fig. 5, where hourly wind speed values at stack release are compared for Exp B and C). Exp A, associated with most dispersed pollutant fields, has significantly lower pollutant air densities, which are for the factor of 0.01 (in the case of maximum 24h averages, Tab. 4) or for the factor of 0.7 (in the case of maximum 1h values, Tab. 3) lower than in Exp B.

Table 3. Comparison of maximum values in the field of 1h daily maximum (shown in Fig. 3) calculated at ground level for SO₂ (in μ gm⁻³). These values present maximum simulated 1h ground level SO₂ values, regardless of the time and location of occurrence.

Table 4. Comparison of maximum values (regardless the location of maximum) in the field of 24h average SO_2 densities (in μ gm⁻³).





Figure 5: Scatter plot comparing hourly wind speed values at location of point source. Comparison between a) experiments B and C and b) experiments B and D is shown separately for winter and summer day.

On the basis of our experiences we can conclude that pollutant densities in Exp A performed with AUSTAL2000 dispersion model may be underestimated also because of the overestimated model plume rise, leading to lower values close to the ground. Based on available data it is hard to conclude which of other experiments may be more in agreement with the true dispersion conditions of the studied days. For diagnostic mass-consistent wind field models it is known that they are able to reproduce wind fields sufficiently well if there are enough reliable measurements available, which was not the case in our study. Only one radiosounding station with vertical atmosphere sounding performed only once a day in the early morning hours is not enough for representation of vertical atmosphere structure throughout the day. Consequently, only three ground meteorological stations (with one, S2, not representative enough to be included in model data assimilation procedures) present data source from which the wind field is constructed in diagnostic meteorological model throughout the day. On the other hand, WRF-Chem model uses archived analyses for boundary and initial meteorological conditions, as well as including different parameterizations, which enable also the simulation of processes (e.g. thermal winds) which cannot be reproduced with diagnostic mass-consistent wind field models (while wind channelling and blocking can be represented in models of both types). But still, to accurately simulate wind fields over complex terrain or otherwise complex area (coastline etc.) remains a challenging issue. In our experiments for two selected days with weak dynamics results of WRF-Chem simulations were quite different between simulations with and without PBL parameterizations, where in simulation without PBL parameterizations simulated winds were too strong. To improve meso-scale meteorological model in such situations with weak dynamics data assimilation or model nudging towards available measurements can be used. This is also one of our plans for future work. Nevertheless, the problem with sparse meteorological measurements available for further evaluation of model results remains unresolved.

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