Mesoscale simulation of meteorological profiles during the Sofia Experiment 2003

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Abstract: Sofia is situated in a mountain valley and suffers from air pollution problems. The planetary boundary-layer-evolution Sofia-Experiment 2003 (comprising radiosoundings every 2 h with vertical resolution 3–4 m) was used to evaluate one configuration of the Weather Research and Forecasting (WRF) model against data. Statistical analysis was performed for each model level and time of radiosounding, as well as for some integral characteristics within the boundary layer. The vertical profiles of relative humidity, temperature, potential temperature, and wind speed were reproduced with correlation coefficient larger than 0.8, while wind direction was poorly resolved up to 1,000 m. The performance of WRF as meteorological driver for air pollution studies was studied separately under convective conditions at afternoon hours (AH, comprising 11, 13, 15, 17 LST) and under transition hours (TH, comprising 09, 11, 19 LST). WRF simulated with smaller bias most of the analysed parameters during TH compared to AH.

Keywords: model evaluation; planetary boundary layer; PBL; consecutive radiosoundings; vertical profiles; mountain valley.

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Ekaterina Batchvarova is a Professor (2010) in Meteorology at NIMH, PhD (1986) and DSc (2007) in Planetary Boundary Layer (PBL) Meteorology. She has published more than 120 papers, 68 of which listed in Web of Science with more than 840 citations and h factor of 18. Her main work is in theory and observations within the PBL, parametrisation of the height of the convective and near neutral PBL, of turbulent fluxes near the ground in boreal forest canopy, dispersion and meteorology in urban conditions, parameterisation of the wind speed profile within the entire PBL for the needs of wind power assessments, etc.

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1 Introduction

The characteristics of the planetary boundary layer (PBL) in particular the vertical profiles of meteorological parameters, predicted by the mesoscale models have to be evaluated for each study area to ensure better air quality forecasts. Larger discrepancies between modelled and observed vertical profiles are reported in complex terrain, coastal and urban conditions, compared to flat homogeneous terrain (Chiao and Dumais, 2013; Doyle et al., 2011; Floors et al., 2013; Gryning et al., 2014; Lupaşcum et al., 2015). Sofia is a large city with complex terrain which experiences air quality problems – smog near the ground during strong inversion situations with shallow PBL in winter and high PM10 concentrations in dry summer periods despite the deep PBL.

Comparing 19 single column models (SCMs) used by major operational numerical weather prediction (NWP) centres and research groups under the first Global Energy And Water Cycle Experiment (GEWEX) atmospheric boundary layer study (GABLS) project, Cuxart et al. (2006) concluded that the operational models produce stronger mixing, resulting in omission of upper inversion development and overestimation of surface friction velocity. Under the second GABLS project, Svensson et al. (2011) and Svensson and Holtslag (2006) documented the intercomparison of 18 SCMs and showed that the models produce divergent results in all compared variables, and that there are noticeable discrepancies between simulated values and observations. These studies found considerable differences between the shape and magnitude of modelled and observed temperature and wind profiles.

The models 3 system (MM5/WRF-SMOKE-CMAQ) is set up for Sofia for a chemical weather forecast (Syrakov et al., 2013). Still, the meteorological fields of this air quality system, as well as the weather forecast using ALADIN, are not validated using upper air observations because in Sofia only one radiosounding per day is performed at 12 GMT (15 LST during daylight saving time). The aim of the present study is to evaluate in detail WRF meteorological profiles against data from consecutive radiosoundings launched every 2 h during daytime (with a 3–4 m vertical resolution) obtained during the Sofia Experiment 2003 (Batchvarova et al., 2006).

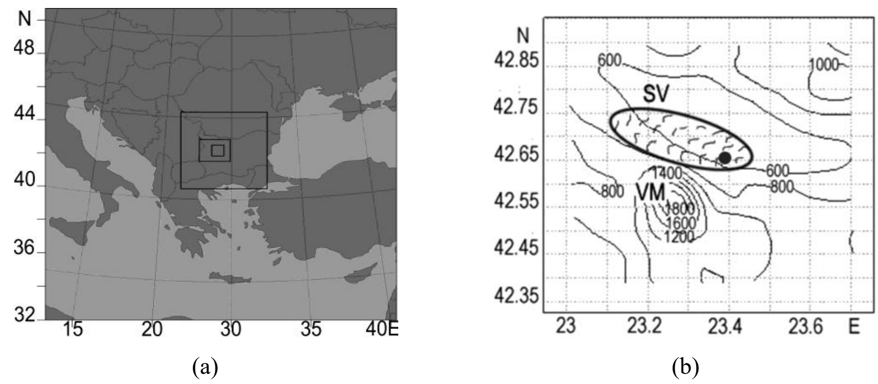
The WRF model (v3.3.1) supports eight PBL first-order or one-and-a-half (and higher) order turbulent kinetic energy (TKE) closure schemes, and numerous combinations with surface layer, surface exchange, and radiation schemes. Therefore, studies comparing the sensitivity of simulated meteorological parameters on PBL scheme are constantly performed (Shin and Hong, 2011). Here, we chose to use a TKE closure Mellor-Yamada-Janjic (MYJ) scheme (Mellor and Yamada, 1982; Janjic, 2002). The local-mixing MYJ scheme was reported by Hu et al. (2010) to simulate higher moisture and lower temperatures, compared to non-local schemes and to perform better for stable and slightly unstable stratifications, compared to free convection conditions. Therefore, it was considered appropriate for early autumn convective conditions in Sofia. Moreover, the experimental profiles used for the evaluation cover the transition periods from stable to convective PBLs in the morning and from convective to stable PBLs in the late afternoon. Thus, the experimental setup allowed to evaluate separately the performance of WRF as meteorological driver for air pollution studies under convective conditions favourable for pollutants dispersion (AH) and under stable to unstable (and opposite) stratification transition (TH), when in addition to conditions unfavourable for dispersion, the morning peak of transport emissions occurs.

This study examines the performance of the WRF model using MYJ PBL scheme compared with data from high resolution in time and height radiosoundings. Section 2 of this paper describes the site and the experimental campaign, while Section 3 introduces the domain configuration and the chosen physical options of the WRF. Model results and evaluation are presented in Section 4, and conclusions are presented in Section 5.

2 Site and experimental campaign

Sofia Valley is situated in Southwestern Bulgaria (Figure 1). The area of the valley is 1,300 km^2. The average altitude above the mean sea level is 550 m. The shape of the valley is oval with a long axis directed from north-west to south-east, with length between 60–70 km and width between 5–30 km. To the north and north-east the valley borders the Balkan Mountain (height up to 1,700 m), and to the south and south-west, the Vitosha Mountain (2,290 m height, a Bulgarian national park) and the Lyulin Mountains. To the east the valley borders the westernmost parts of the Sredna Gora Mountain (up to 1,300 m) and to the west, the Slivnitsa Heights (700–800 m).

Figure 1 (a) Domain configuration (b) terrain heights in domain 4



Notes: Where SV – Sofia Valey, VM – Vitosha mountain, oval is area of Sofia City, and black dot marks NIMH location.

The population density of the entire valley is roughly 1,100 people km^{-2}, while the population density of the city is 2,600 people km^{-2}, following information from Official Census (2011). The number of registered cars in Sofia city is about 1,000,000 which accounts for high transport emissions of PM, NOx, etc. Presently, there are three big natural gas thermal power plants with tall stacks and no other big industrial sources of

NOx. The complex terrain features and the high level of urbanisation result in complex multilayer structure of the PBL which is a challenging task for models. The reliable simulation of PBL parameters is of crucial importance for air quality modelling applications. It is important that meteorological models reproduce adequately the meteorological fields, especially when such models are part of air quality modelling systems (AQMS).

The 'Sofia Experiment 2003' field campaign was carried out in early autumn 2003, 27 September to 3 October (Batchvarova et al., 2006). During the experimental campaign, 35 soundings were performed to document convective boundary layer development. Seven sondes were launched from the National Institute of Meteorology and Hydrology (NIMH) on each day of the campaign, starting at 7 am and ending at 7 pm LST. NIMH is located in the Mladost district in the south-east part of the city [Figure 1(a)]. For westerly and northwesterly flows, the measurements at this site represent urban conditions, while for southerly and easterly flows they represent mixed suburban and rural conditions. The studied period covered days with a well-developed convective boundary layer. The soundings were performed with 2 h temporal resolution and increased vertical resolution as the ascend velocity was kept to about 3–4 m s^{-1} (two times slower than standard radio sounding). The collected data set of intensive observations comprises vertical profiles of air temperature, humidity, and wind speed and direction and is used in our study for WRF model performance evaluation.

3 Method

Numerical simulations were performed using the Advanced Research core of the weather research and forecasting (WRF) model, version 3.3.1 (Skamarock et al., 2008). The model was initialised with the US National Center for Environmental Prediction Final Analyses (FNL) with 1 × 1 degree spatial and 6 h temporal resolution. WRF was run with two-way nesting on four domains with horizontal grid resolution of 36, 12, 4, and 1.33 km; horizontal grid dimensions of 58 × 58 (domain1, D1 – the outermost), 43 × 43 (D2), 37 × 34 (D3), and 43 × 43 (D4) points, respectively [Figure 1, (b)]; and with 26 vertical levels up to 50 hPa. These four domains were located in such way that the finest domain contained SV and VM, and was centred at the location of the radiosounding site (23.38°E, 42.65°N) or D4 (x = 23, y = 22).

The parameterisations of cloud physics used were Thomson graupel for D3, D4 (Thompson et al., 2004), and WRF single-moment five-class (Hong et al., 2004) for D1 and D2; RRTM (Mlawer et al., 1997) for longwave radiation; Goddard (Chou and Suarez, 1994) for shortwave radiation; MYJ TKE scheme for PBL; Noah LSM (Chen and Dudhia, 2001) for land surface; and Janjic-Eta surface layer scheme (Janjic, 1996, 2002) for the surface layer. The Grell3D (improved version of Grell and Devenyi, 2002) cumulus parameterisation was used only for D1 and D2. The selection of the parameterisation was based on the characteristics of the schemes reported in detail by Skamarock et al. (2008) and on their computational cost.

The period 27 September to 3 October (168 h) was simulated by two runs with run duration of 84 h, starting at 12 GMT. The first 16 h were not used for evaluation and were considered as spin-up time.

The performance of the presented configuration is evaluated using the following statistics: mean, bias (model – measurement), root-mean-square error – RMSE, standard deviation – SD, and correlation coefficient – r. The studied parameters are temperature (T), potential temperature (Θ), relative humidity (RH), mixing ratio (MR), and wind speed (WS). Calculations are performed for the period 28 September 28 to 3 October 2003 using data from 35 soundings and corresponding model results at 19 model levels up to 8,000 m which provides 665 pairs for analysis. The observation data were interpolated to the height of the model levels.

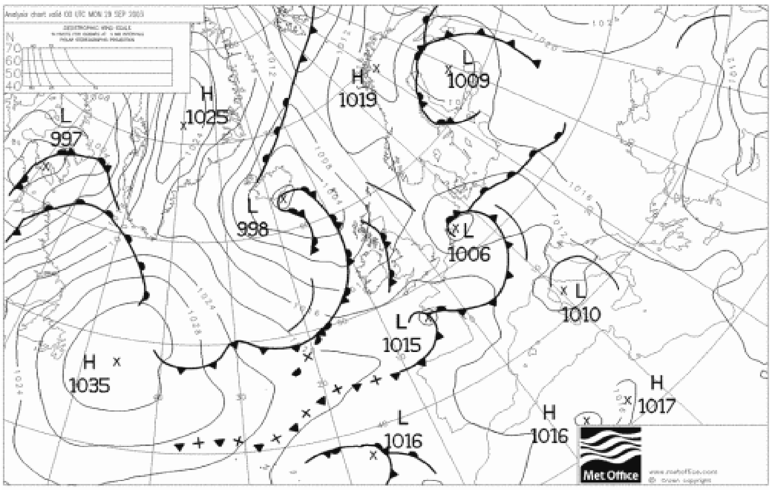
To examine the way WRF (in the configuration presented above) reproduces the structure of the PBL over Sofia, we compare all modelled to measured parameters for the entire period of 'Sofia Experiment 2003' for each radiosounding and for all model levels (Figure 3). The profiles at convective (15 LST) and stable (19 LST) conditions near the ground demonstrate the performance of the MYJ PBL scheme under different stratification (Figure 4). As the dates 29 September and 3 October 2003 feature weak anticyclone pressure fields with no frontal events, they are characterised by no obstructions for development of convective boundary layer. On these dates the boundary layer develops from destruction of the morning ground-based inversion, passing through fully developed convective layer in the afternoon to collapse and stable stratification near the ground during the evening transition period. The difference between the days is in wind direction: westerly-northwesterly flow on 3 October 2003 and easterly on 29 September 2003 representing urban and mixed suburban and rural conditions, respectively.

For further analysis, the 665 pairs are divided into two groups: transition hours (TH) covering model output vs. measurements at 07, 09, 19 LST and afternoon hours (AH) covering model output vs. measurements at 11, 13, 15, 17 LST. This separation was introduced to distinguish the model performance under transition and convective conditions, which is important information when using WRF as meteorological driver for AQ simulations.

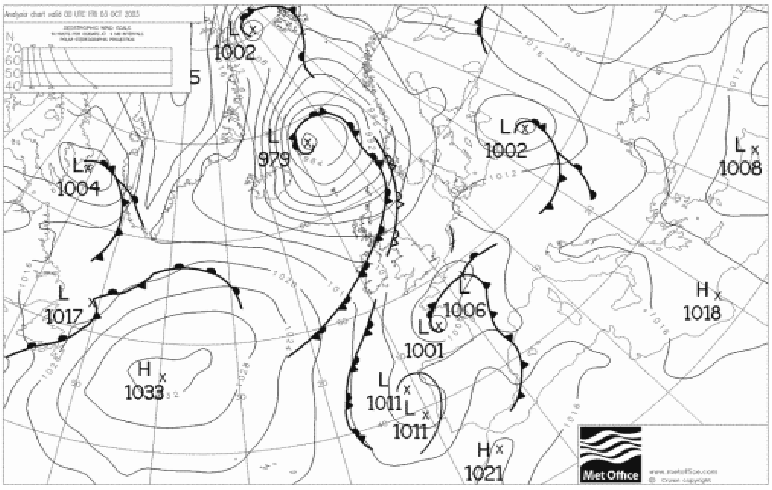
4 Model results and evaluation

During the 'Sofia Experiment 2003' the synoptic conditions were characterised by weak anticyclonic pressure field near the ground, warm and sunny weather during 27–29 September and 2–3 October. On 30 September a cold front passed over Bulgaria and rain of 2.6 mm was reported for Sofia on 1 October. Figure 2 illustrates the difference in circulation on 29 September and 3 October. Other maps from the archive (not included here) show that on 29 September, the surface pressure field is characterised by very low pressure gradient, with very dry air mass in the upper layers and weak southerly wind. On 3 October, the surface pressure gradient is still low but in the upper layers the region is in the southern periphery of a low pressure system, much more humid air at the upper layers, and westerly circulation in these layers. Figure 4 shows that 3 October was warmer, with lower wind speed and representing urban conditions as the flow was mainly from NW, compared to 29 September when the flow was from S and SE (rural and suburban conditions).

Figure 2 UK Met Office surface weather maps at (a) 00 GMT for 29 September 2003 and (b) 3 October 2003)



(a)



(b)

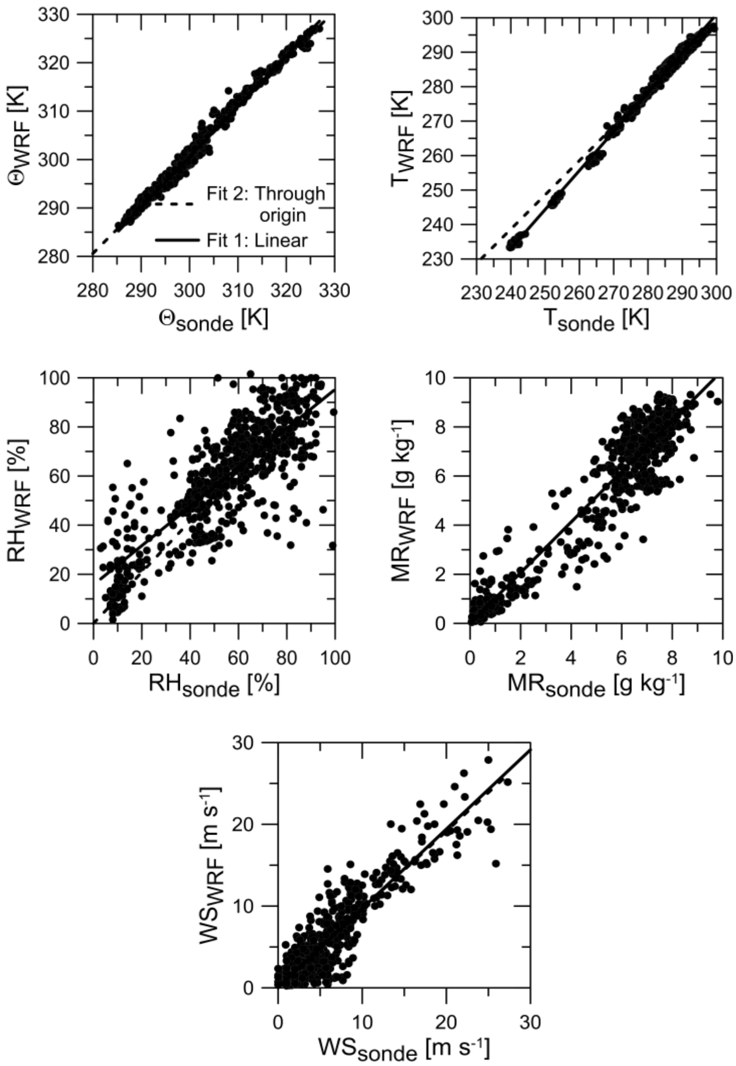
Source: Met Office Archive (http://www.wetterzentrale.de/topkarten/)

Table 1 Summary statistics (using integrated data up to 8,000 m) for all radiosoundings

	T [K]	*Θ [K]*	*RH [%]*	*MR [g kg^{-1}]*	*WS [m s^{-1}]*
MeanWRF	277.9	302.6	58.6	5.3	5.4
Bias	–1.7	0.7	4.8	0.2	–0.1
RMSE	2.7	1.4	14.7	1.0	2.2
SD	2.2	1.2	13.9	0.9	2.2
r	0.99	0.99	0.82	0.95	0.90

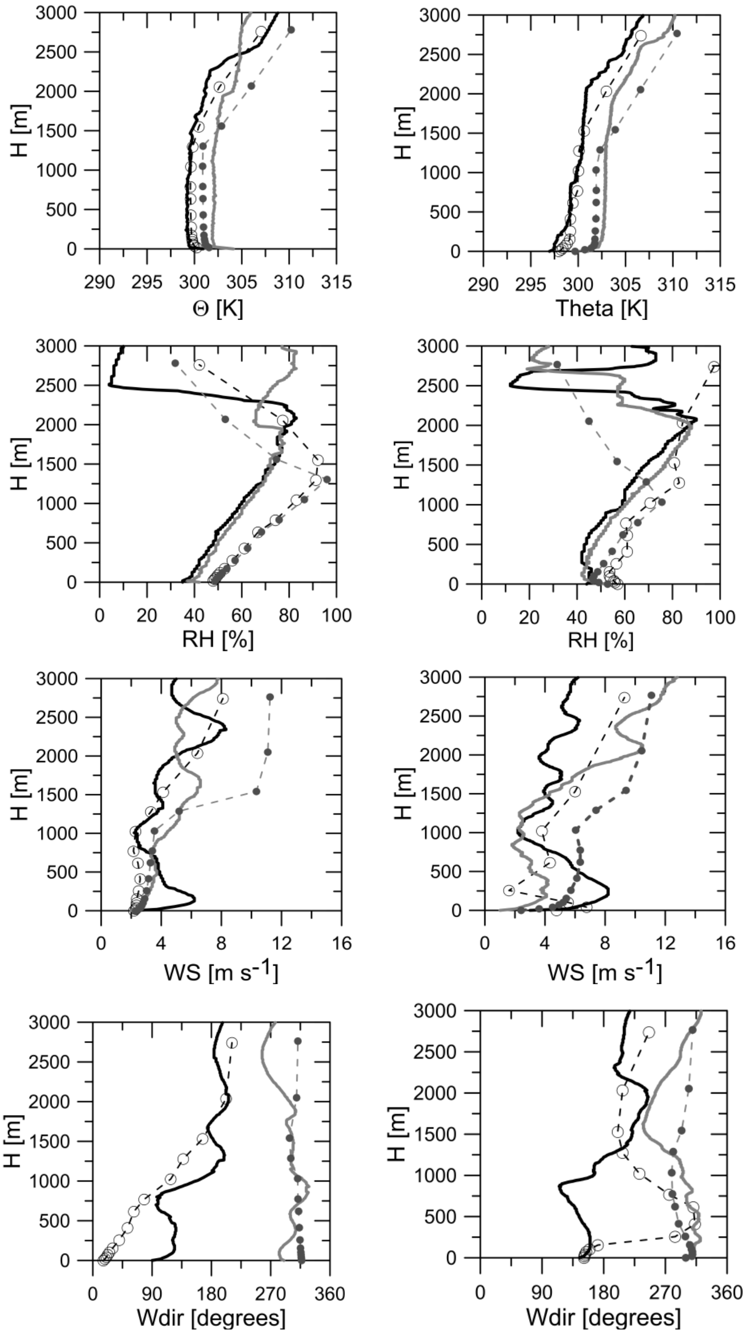
Note: All statistical and meteorological parameters are defined in text.

Figure 3 Scatter plots of Θ, T, RH, MR, WS for all radiosoundings and all levels up to 8,000 m; all symbols are defined in text



The evaluation of the model performance for all observational times (35 soundings) and heights up to 8,000 m (19 model levels) is given in Table 1. There is positive extremely strong ($0.8 < r < 1$) correlation between model and measurements for all studied parameters. The relatively lower r values for RH are attributed to the local mixing in MYJ scheme. Slight underestimation of temperature (bias = –1.7 K) and wind speed (bias = 0.1 m s^{-1}) and overestimation of potential temperature (bias = 0.7 K), MR (bias = 0.2 g kg^{-1}) and RH (bias = 4.8 %) can be noted. The most dispersed parameters are MR, WS and RH (Figure 3).

Figure 4 Comparison between measured and modelled parameters at (a) 15 and (b) 19 LST on 29 September and 3 October 2003



Hu et al. (2010) discussed that the local closure MYJ scheme fails to entrain adequately drier and warmer air from the surface higher up in the PBL which we also observe in RH, but not in temperature. In fact, temperature profiles (not presented here) and potential temperature profiles are the closest profiles to the observed ones (Figure 4). Vertical profiles of potential temperature at 15 LST are nearly constant with height as expected during daytime in well-mixed PBL (Srinivas et al., 2007) with height of 1,500 m in these cases. Wind speed is underestimated by the model close to the ground. Wind direction is better resolved on 3 October, the day when the variability of wind direction from radiosounding data with height was smaller. Wind direction on 29 September is easterly in the morning corresponding to rural and suburban conditions and changes to southerly from suburban areas, whereas on 3 October it is westerly corresponding to urban conditions [Figure 1(a)].

Figure 5 Averaged value of Δ (Δ = Valuem-Valueo) from all 35 soundings and its SD for each model level up to 8,000 m

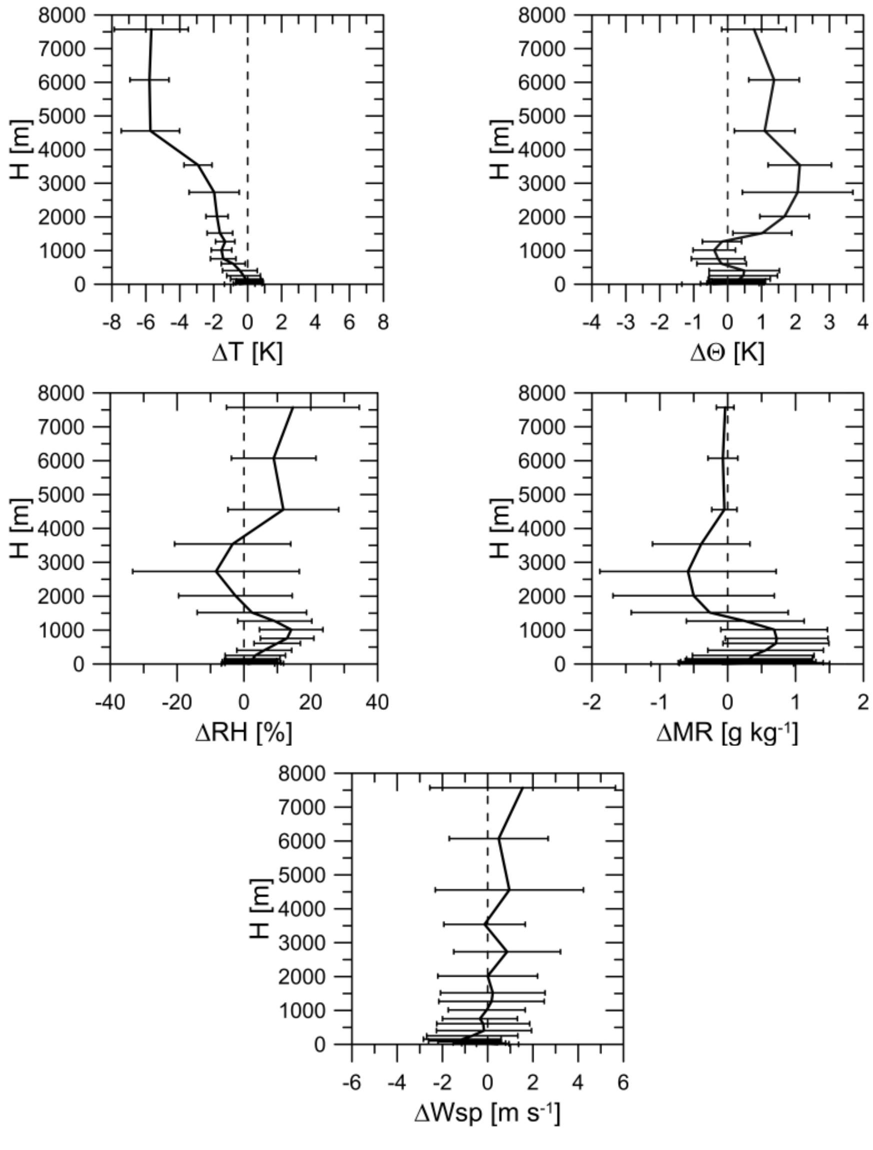


Figure 5 shows the change with height of the mean difference between modelled and measured parameters and its standard deviation based on all 35 soundings. The largest underestimation of T (with 6 K) is observed between 4,500–8,000 m. The potential temperature is slightly over-predicted near the ground (with 0.5 K) and above 1,500 m (2 K). Over-estimation of RH is obtained below 1,700 m and above 4,000 m with maximum of 20 % around 1,000 m and 7,600 m. In the first 1,200 m MR is over-predicted by 0.75 g kg^{-1}. Higher up, MR is under-predicted of the same magnitude. In the layer 4,500 m – 8,000 m the simulated values of MR almost coincide with the measured ones. WS is underestimated up to 1.2 m s^{-1} in the first 1,000 m and is overestimated up to 1.7 m s^{-1} higher up.

Table 2 Summary statistics (using integrated data up to 8,000 m) for TH and AH (units as in Table 1)

	TH (07, 09, 19 LST)					*AH (11, 13, 15, 17 LST)*				
	T	*Θ*	*RH*	*MR*	*WS*	*T*	*Θ*	*RH*	*MR*	*WS*
Mean WRF	277.4	301.3	62.3	5.3	5.4	*279.0*	*303.1*	*55.9*	*5.5*	*5.1*
Bias	–1.6	0.8	3.3	0.04	–0.1	*–1.7*	*0.7*	*5.2*	*0.3*	*0.1*
RMSE	2.7	1.4	15.2	0.9	2.5	*2.8*	*1.5*	*14.9*	*1.1*	*1.9*
SD	2.4	1.2	14.9	0.9	2.5	*2.2*	*1.4*	*13.9*	*1.1*	*1.9*
r	0.99	0.99	0.82	0.95	0.88	*0.99*	*0.99*	*0.78*	*0.94*	*0.92*

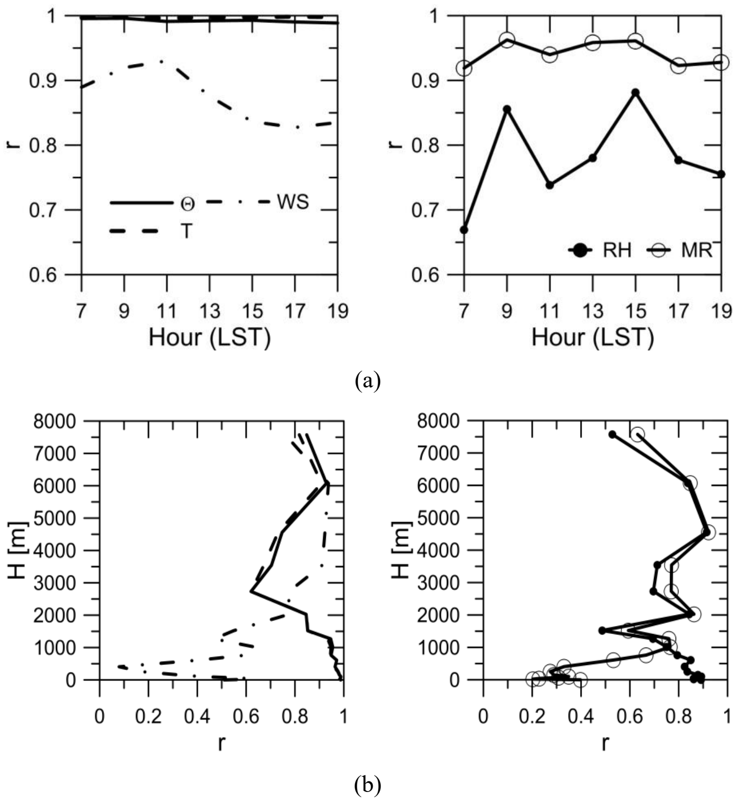
Note: All statistical and meteorological parameters are defined in text.

The calculated separate analysis for TH and AH values of *r* (Table 2) for all parameters shows a strong (0.60–0.80) or extremely strong relationship (0.80–1.0) between observed and modelled values. WRF performance is slightly better in TH than in AH, except for wind speed. WRF tends to overestimate Θ, RH, MR and WS for AH (bias > 0), underestimate T for AH and TH and WS for TH (bias < 0). Based on this statistics for all model levels and observation times, we consider that the used WRF configuration performs better for temperature than for moisture and wind speed.

Figure 6 (upper panels) shows the diurnal change *r* averaged for all model levels. Almost constant high values of *r* are calculated for temperature parameters, while *r* for wind speed and moisture parameters shows distinct diurnal pattern and lower values.

The reconstruction ability of this WRF configuration to reproduce vertical PBL structure, Figure 6(b), is examined by comparing the model output at each level with measurements from all 35 radiosoundings up to 8,000 m. There is strong correlation ($r >$ 0.6) between output from WRF and measurements for Θ and T for all levels up to 8,000 m, the lowest value for *r* being calculated at height about 2700 m. There is extremely strong positive correlation ($r > 0.8$) for T and Θ up to 1,200 m, as well as for two of the higher levels about 6,000 m and 7,600 m. Strong to extremely strong correlation is observed for RH values except at height about 1,500 m ($r = 0.48$). MR is simulated with $r < 0.5$ up to 250 m and with $r > 0.5$ for the higher levels. The lowest values of $r(r < 0.5)$ for wind speed are between 100 m and 600 m and at height 1,270 m, while for the rest levels $r > 0.5$.

Figure 6 (a) Variation of correlation coefficient *r* with time, averaged for all model levels up to 8.000 m (b) Variation of correlation coefficient *r* with height, averaged for all times of radiosoundings



5 Conclusions

The PBL at a site, which is representative for rural, suburban or urban conditions depending on wind directions and which is situated in a mountainous valley, was simulated with WRF (ARW) v3.3.1 and modelled profiles were evaluated against radiosounding data collected during the ‘Sofia Experiment 2003’. The radiosoundings were performed with 3–4 m resolution in height, every 2 h starting at 7 LST and ending at 19 LST, during five days.

The set up of WRF (with MYJ PBL) simulated sufficiently well the vertical profiles of temperature, potential temperature (< 2 K) and RH (< 20 %) within the PBL. On 3 October, below 1,500 m, the wind speed was reasonably resolved at 15 LST while above this height it was overestimated. At 19 LST on the same date the entire wind speed profile was overestimated. On 29 September at heights below 1,500 m, the wind speed was underestimated and its characteristic maximum was not resolved. Within the lowest 1,000 m, the wind direction was poorly simulated. The overall performance of the model, based on data set formed by all WRF levels (up to 8,000 m) and all times of radiosoundigs, showed extremely strong positive correlation (0.82–0.99) for T, Θ, RH, MR and WS.

The profile of the correlation coefficient (comparison between model and observations for all 35 soundings at each model level) revealed lower correlation ($r < 0.6$) for WS and MR within the first few hundred metres and higher correlation ($r > 0.80$) above 2,000 m. For temperature, extremely strong correlation ($r > 0.8$) was obtained below this height and above 5,000 m. The temporal variations of all studied parameters, except RH, were reconstructed by the model with extremely strong correlation to observations. For RH, strong correlation was obtained.

The purpose of this analysis was to demonstrate the ability of WRF to simulate adequately meteorological fields in the vertical direction with emphasis on PBL in order to support studies with Models 3 system used for operational air pollution forecast in Sofia. WRF simulated T, Θ, RH and MR with smaller bias and higher correlation coefficient during the transition periods than in the afternoons, while for WS r was slightly greater in the AH. In this way, we show that the meteorological factor in forecasting concentrations during TH (when peak in transport emissions occurs as well) is adequately resolved.

We plan to perform extensive observations on the vertical structure of meteorological parameters in different seasons in Sofia and its surroundings to obtain further insight into the difference between urban and rural conditions. The present configuration of WRF as well as other configurations of its will be tested on the new data sets to study the sensitivity to PBL schemes and the spatial resolution.

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