VALIDATION OF MIXED LAYER HEIGHTS AND AEROSOL CONCENTRATIONS SIMULATED WITH WRF-CHEM

Renate Forkel, Klaus Schäfer, Stefan Emeis

Karlsruher Institut für Technologie (KIT), IMK-IFU, Garmisch-Partenkirchen, Germany

Abstract: Mixed layer heights from ceilometer measurements within the region of Augsburg (Southern Germany) are used to evaluate boundary layer heights from WRF/Chem simulations for a winter time situation. A comparison of the YSU and the MYJ boundary layer schemes indicates that the simulated daytime boundary layer height is too low for the YSU scheme.

Key words: *Mixed layer height, ceilometer, WRF/Chem.*

INTRODUCTION

An important factor influencing the near surface concentrations of pollutants is the height of the mixed layer. This was demonstrated on the basis of measurements in Hanover within the time frame from October 2001 to April 2003 (Schäfer *et al.*, 2006). The influence of mixed layer height (MLH) on NO_x concentrations measured at a roof top station is shown in Figure 1.

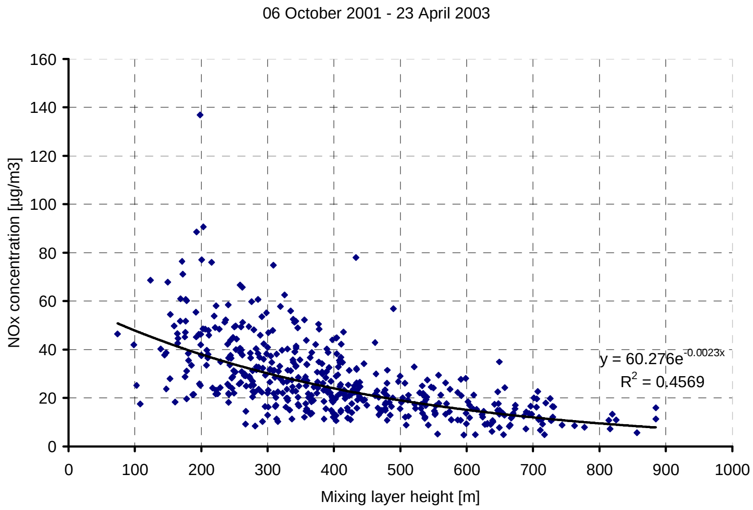

Figure 1. Exponential relationship for NO_x concentration with mixing layer height (MLH) from SODAR for the roof-top station at the street canyon Göttinger Strasse in Hanover (urban background, one-hour mean data) during a long-term study together with the square of the correlation coefficient R^2.

However, particularly during winter time mixed layer height and vertical exchange are still a crucial point of model simulations. The use of radiosonde data only permits validation of modeled mixing layer heights at selected times. However, ceilometers permit the continuous observation of the mixed layer height.

Ceilometer measurements from a long term campaign within the region of Augsburg (Southern Germany) were used for the validation of modeled boundary layer heights from a WRF/Chem (Grell *et al.*, 2005) simulation. Additional observational data such as temperature profiles, wind, and concentrations of gaseous pollutants and particulate matter are also included for the model validation.

MEASUREMENTS AND MODEL SETUP

Measurements

The city Augsburg (ca. 265000 inhabitants) is situated in Southern Germany about 60 km West-North-West of Munich in a rural area. The measurement site for the determination of the mixing layer height (MLH) with a remote sensing device and particle characteristics is placed on the campus of the University of Applied Sciences Augsburg which is approximately 1 km to the South-East of the city centre. Within a radius of 100 m it is surrounded by campus buildings, a tram depot and a small company. The nearest main road is in the North-East at a distance of 100 m. Within a radius of approximately 200 m the monitoring site is almost completely surrounded by residential areas, apart from a small park located in a north-western direction.

Due to the importance of continuous availability of MLH and layering data for the lower atmosphere ceilometers have been operated since 2006. This optical remote sensing technique provides particle backscatter intensities of an emitted laser beam in the near infrared spectral range and adds information about the height-dependant aerosol concentration; gradient minima within this profile mark the borders of mixed layers. The performance of the ceilometers, which are originally used to investigate cloud layers, vertical visibility, and cloud cover, is sufficient to determine convective layer depths exceeding 2000 m. It enables the detection of nocturnal stable layers down to 150 m (Vaisala LD40) or 50 m (Vaisala CL31). The instrument runs in fully automated, hands-off operation mode. Laser power and window contamination are permanently monitored to

provide long-term performance stability. The heights of the near surface aerosol layers and the MLH are analyzed from optical vertical backscatter profiles. Here the gradient method is used (Münkel, 2007). A second ceilometer is operated at the Northern edge of the city since 2007.
The further remote sensing instrumentation for continuous determination of MLH which is operated in Augsburg is SODAR (sound detection and ranging) and RASS (radio-acoustic sounding system). MLH is determined solely from Metek SODAR data as the minimum of the height of the ground-based echo layer and the height of an elevated echo maximum (if present). An intercomparison between these three remote sensing techniques is given in Emeis *et al.* (2004). The SODAR discerns strong vertical thermal gradients and temperature fluctuations connected to turbulence and the Metek RASS provides via the determination of the speed of sound a nearly direct measurement of the vertical temperature profile up to about 500 m above ground.

Model

The simulations with WRF/Chem were carried out for three nested domains with horizontal resolutions of 36 km, 9 km, and 2.25 km. The boundary conditions for the first model domain are based on the 6-hourly NCEP FNL operational global analysis data with 1°x1° horizontal resolution. The following example was taken from a simulation of the first decade of January 2009. The model was set up with WSM 6-class microphysics, the NOAH land surface model, RADM2 gas phase chemistry and MADE/SORGAM aerosol module, and alternatively with the YSU (Yonsei University) boundary layer scheme (Hong *et al.*, 2006) and the Mellor-Yamada-Janijic boundary layer scheme (Janjic, 2002).
In the case if the YSU boundary layer scheme the boundary layer (PBL) height is a critical factor for the determination of the turbulent exchange coefficient. In the mixed layer case it is determined using a critical bulk Richardson number of zero in a two step procedure as the first neutral level by checking the stability between the lowest model level and levels above considering the temperature perturbation due to surface buoyancy flux. The Mellor-Yamada-Janijic boundary layer scheme is a Level 2.5 turbulence closure TKE (turbulent kinetic energy) based scheme. The PBL height is determined as the height where $TKE^{1/2}$ falls below a critical value of 0.001 $m^2\ s^{-2}$.

RESULTS

The meteorological situation at Augsburg during the considered episode was characterized by north-easterly winds, temperatures between -2 and -15 °C, and frequent occurrences of fog and high fog situations. Generally the ceilometer measurements showed only small differences between the mixed layer heights at the sites South-East of the city and North of the city. The mean difference in January 2009 was on the order of 10%, the maximum difference of 80 m was observed in the afternoon of January 26th. This indicates that the observed mixing layer heights can be considered as representative for a model grid area.

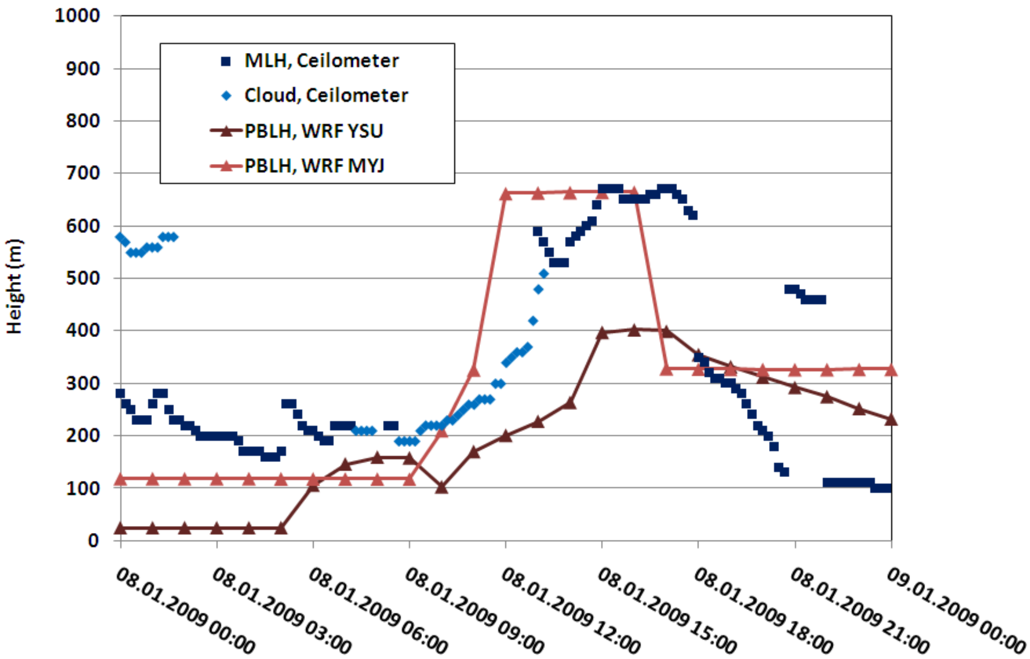

Figure 2. Comparison of observed and simulated mixed layer heights for January 8th 2009.

On January 5 to 7 cloudy conditions were prevailing, which was only partly reproduced by the model simulations. Generally, the existence and life time of shallow cloud and fog layers during winter situations with low wind speeds is difficult to reproduce by any model. The ceilometer measurements also show cloud layers and practically no mixed layer for these days. For both boundary layer schemes, the observed cloudy conditions were only reproduced for January 5th. Only small patches with cloud cover outside the Augsburg region were simulated for January 6th and 7th. As a consequence the simulated night time temperatures were too low for the night following January 6th. Therefore, near surface NO_x mixing ratios were overpredicted by almost a factor of two for this particular night and consequently simulated ozone mixing ratios were too low as compared to the observations at the air quality monitoring station located at the southern boundary of Augsburg (http://www.lfu.bayern.de/luft). Most of the time, the course of the simulated PM10 agrees well with the observed course for both PBL physics although the peak concentrations are underestimated by the model. Generally, observed as well as simulated PM10 shows less pronounced temporal fluctuations than NO_2 and is less susceptible to short term local effects. This can be attributed to the significant amount of secondary aerosol material which shows a lower temporal and spatial variability than the primary compounds. The model results indicate that up to 40% of the PM2.5 mass consists of secondary aerosol material.

For clear conditions or days with dissolving cloud layers, a comparison between the observed and simulated development of the mixed layer height is possible. In agreement with the results of Borge *et al.* (2008) the YSU boundary layer scheme results in too low PBL heights as compared to the MLH from the ceilometer measurements (Figure 2). The simulations based on MYJ boundary layer scheme generally resulted in a higher boundary layer. The shape of the temporal course during daytime is better represented for the YSU boundary layer scheme.

However, the observed sudden drop of the mixed layer height to a height of 100 m in the evening hours of January 8th and the subsequent fog formation on January 9th is not reproduced by the simulations which results in an under prediction of NO_x and PM concentrations during this night.

SUMMARY

Mixed layer heights from long term ceilometers measurements near Augsburg were compared against model simulations with WRF/Chem for a winter time situation. Ceilometer measurements permit a continuous evaluation of the simulated development of the mixed layer. The occurrence of fog and high fog situations and shallow cloud layers and their representation in model simulations remains a crucial point for air quality simulations during winter time. It determines critically whether a realistic course of the MLH and resulting simulated pollutant concentrations can be reproduced by WRF/Chem.

REFERENCES

Borge, R., V. Alexandrov, J. del Vas, J. Lumbreras, E. Rodríguez, 2008: A comprehensive sensitivity analysis of the WRF model for air quality applications over the Iberian Peninsula. *Atmos. Environ.*, **42**, 8560-8574.

Emeis, S., C. Münkel, S. Vogt, W. Müller and K. Schäfer, 2004: Determination of mixing-layer height. *Atmos. Environ.*, **38**, 273-286.

Grell, G. A., S. E. Peckham, R. Schmitz, S. A. McKeen, G. Frost, W. C. Skamarock and B. Eder, 2005: Fully coupled “online” chemistry within the WRF model, *Atmos. Environ.*, **39**, 6957–6975.

Hong, S.-Y., Y. Noh, J. Dudhia, J., 2006: A new vertical diffusion package with an explicit treatment of entrainment processes. *Monthly Weather Review*, **134**, 2318–2341.

Janjic, Z.I., 2002. Nonsingular Implementation of the Mellor – Yamada Level 2.5 Scheme in the NCEP Mesomodel, *NCEP Office Note*, **437**, 61 pp.

Münkel, C., 2007: Mixing height determination with lidar ceilometers - results from Helsinki Testbed. *Meteorol. Z.*, **16**, 451-459.

Schäfer, K, S. Emeis, H. Hoffmann and C. Jahn, 2006: Influence of mixing layer height upon air pollution in urban and sub-urban areas, *Meteorol. Z.*, **15**, 647-658.