COST 728/MESOSCALE MODELLING: EVALUATION STUDIES SESSIONS

EVALUATION OF A SEVERE AIR QUALITY EPISODE IN HELSINKI IN AUGUST 2006, CAUSED BY REGIONALLY TRANSPORTED SMOKE
M. Rantamäki, M. Sofiev, N. Eresmaa, S. Saarikoski, T. Mäkelä, R. Hillamo, A. Sarkanen, J. Kukkonen and A. Karppinen - Finnish Meteorological Institute (FMI)

PERFORMANCE OF MODELS-3/CMAQ FOR PREDICTING URBAN AND REGIONAL CONCENTRATIONS OF O_3 AND NO_2 DURING A SUMMER EPISODE IN THE SOUTHEAST OF ENGLAND, UK
Y YU[1], N Kitwroon[1], R S Sokhi[1], D R Middleton[2] and B Fisher[3] - [1]Centre for Atmospheric and Instrumentation Research (CAIR), University of Hertfordshire, Hatfield, Hertfordshire, AL10 9AB, United Kingdom, [2]Met Office, FitzRoy Road, Exeter EX1 3PB, U.K, [3]Environment Agency, Reading, RG1 8DQ, U.K.

EVALUATION OF THE INFLUENCE OF WILD LAND FIRES ON AIR QUALITY IN CITIES – COMBINED UTILISATION OF GROUND- AND SATELLITE-BASED OBSERVATIONS AND MODELLING
Jaakko Kukkonen; Sanna Saarikoski; Markus Sillanpää; Hilkka Timonen; Karri Saarnio; Kimmo Teinilä; Mikhail Sofiev; Ari Karppinen; Risto Hillamo - Finnish Meteorological Institute

ACCOUNTING FOR SMALL-SCALE EMISSION AND CONCENTRATION VARIABILITY IN AIR QUALITY MODELS
S. Galmarini[1], J.-F. Vinuesa[1] and A. Martilli[2] - [1]Institute for Environment and Sustainability European Commission, DG-Joint Research Centre, TP 441, 21020 Ispra - Varese (Italy), [2] CIEMAT, Madrid, Spain.

BOUNDARY CONDITIONS AND THEIR IMPACT ON URBAN SCALE CTM SIMULATIONS
Douros I.[1], Naneris C.[1], Tsegas G.[1], Schaap M.[2] and Moussiopoulos N.[1] - [1] Aristotle University of Thessaloniki, Laboratory of Heat transfer and Environmental Engineering, Box 483, Aristotle University, Gr-54124, Thessaloniki, Greece, [2] TNO, Environmental Quality Department, P.O. Box 342, 7300 AH, Apeldoorn, The Netherlands

EFFECTS OF DIFFERENT SURFACE PARAMETERIZATIONS ON MODEL PERFORMANCE IN URBAN AREAS
Sylvia I. Bohnenstengel[1], K. Heinke Schlünzen[2] - 1) Max-Planck-Institut für Meteorologie, ZMAW, Hamburg, Bundesstr. 53, 20146 Hamburg, Germany, 2) Meteorologisches Institut, ZMAW, Universität Hamburg, Bundesstr. 55, 20146 Hamburg, Germany

INFLUENCE OF DIFFERENT PBL SCHEMES ON OZONE PREDICTIONS OVER THE GAA
[1]Elissavet Bossioli, [1]Maria Tombrou, [1]Aggeliki Dandou, [1]Eleni Athanasopoulou, [1]Kostas V. Varotsos - [1]National and Kapodistrian University of Athens, Department of Physics, Division of Applied Physics, Laboratory of Meteorology

Proceedings of the 6th International Conference on Urban Air Quality
Limassol, Cyprus, 27-29 March 2007

EVALUATION OF A SEVERE AIR QUALITY EPISODE IN HELSINKI IN AUGUST 2006, CAUSED BY REGIONALLY TRANSPORTED SMOKE

M. Rantamäki, M. Sofiev, N. Eresmaa, S. Saarikoski, T. Mäkelä, R. Hillamo, A. Sarkanen, J. Kukkonen and A. Karppinen

Finnish Meteorological Institute (FMI)

ABSTRACT
The summer of 2006 was exceptionally dry in the areas surrounding the Gulf of Finland; this resulted in frequently occurring wild land fires, especially in Russia and Estonia. The regionally transported smokes emitted by biomass burning had a strong impact on the $PM_{2.5}$ mass concentrations in Helsinki from 18 July to 28 August, 2006; the $PM_{2.5}$ concentrations were especially high from 7 to 28 August. The concentrations of $PM_{2.5}$ were substantially also elevated at regional background stations in Southern Finland. The air quality modelling system SILAM was used for the forecast of the $PM_{2.5}$ concentrations generated by wildland fires. The emission fluxes of $PM_{2.5}$ from wildland fires were evaluated based on the MODIS temperature anomalies. The SILAM model forecasted well the overall temporal and spatial distribution of the concentration plumes; however, the absolute values of the fine particular matter concentrations were underpredicted, most likely due to inaccuracies in the emission modelling.

1. INTRODUCTION

Land and forest fires (collectively referred to as wildland fires) have serious negative impacts on human safety, air quality and health, regional and global climate change and regional economies (e.g., tourism, transport, aircraft operations). Forest fires can substantially increase the regional scale emissions of greenhouse gases and particulate matter into the atmosphere, especially during spring and summer.

Fires produce a wide range of harmful or hazardous pollutants, including fine particles that can be transported all over Europe, where they can constitute a serious health risk for the population. For quantitative information of the effects of wildland fires, accurate estimates are needed (i) on the size of the burning area, (ii) the fire intensity and initial elevation of the plume, (iii) the emissions of particulate matter and gaseous pollutants, (iv) the transport and evolution of the resulting pollutant plume.

2. MATERIALS AND METHODS

2.1 Meteorological conditions and observations

Almost during the whole August of 2006, there was a center of high pressure near Kola Peninsula, and easterly winds prevailed in Southern Finland and Estonia. In the northern parts of Finland, precipitation rates were near normal, while in the areas surrounding the Gulf of Finland and on the coast of the Gulf of Bothnia, precipitation rates were only a fraction of the normal rate. These weather conditions allowed air masses polluted with the smoke originating from numerous wild land fires in Russia and Estonia to be transported to the Eastern and Southern parts of Finland and subsequently, to Central Finland and to the coast of Gulf of Bothnia.

In the Helsinki metropolitan area, a dense meteorological observation network “Helsinki Testbed” (http://testbed.fmi.fi) has been implemented by The Finnish Meteorological Institute (FMI) and Vaisala Oyj for two years, from 2005 to 2007. We have utilized the observations from the network in analyzing this episode. Besides numerous other measurement systems, the network contains seven ceilometers; radiosoundings are also performed occasionally. The measurements are performed at six different locations: 2 urban, 2 suburban and 2 rural sites.

As aerosol concentrations are commonly lower in the free atmosphere than in the mixing layer, the mixing height (MH) can be associated with a strong gradient in the vertical backscattering profile. In order to interpret the ceilometer data, we have used a 3-step idealized profile method, where an idealized backscattering profile is fitted to the measured profile, and the middle step indicates the mixing height. This method is an extension of the original (1-step) idealized profile method, originally described by Steyn et al. (1999). The soundings have been treated in two ways: In all cases we have determined the mixing height using the Richardson method (Joffre et al., 2001), and additionally we have also scrutinized the daytime soundings with the Holzworth method (Holzworth 1964, 1967)

2.2 Concentrations

The fine particle concentrations were high from 18 July to 28 August. Concentrations were also high at the regional background stations of Virolahti and Utö. At the urban background station of Kumpula in Helsinki, the $PM_{2.5}$ and $PM_{2.5-10}$ mass concentrations were measured with two Tapered Element Oscillating Microbalance units (TEOM). Size range was selected using a virtual impactor (VI). The chemical composition of fine particles was determined simultaneously with the $PM_{2.5}$ mass concentration measurements during the episode. This data is presented elsewhere (Saarikoski et al., 2006) and is not shown here. Similar analyses were performed previously for an episode caused by wildland fires in the spring of 2006 (Saarikoski et al., 2007).

Based on data from the MODIS instrument onboard the NASA Aqua and Terra satellites, the nearest wild land fires were located at distances of 100 – 200 km from Helsinki. The $PM_{2.5}$ concentrations were frequently high between 7 and 16 August, 2006 (Fig. 1). The highest $PM_{2.5}$ values in Helsinki were measured on August 21, when the highest hourly mean value of $PM_{2.5}$ was almost 180 µg/m^3. Typical yearly average $PM_{2.5}$ concentration in Helsinki is 8 µg/m^3. During the most polluted hours, visibility was poor in many places in the Southern Finland and the Gulf of Finland; this also caused difficulties to marine traffic.

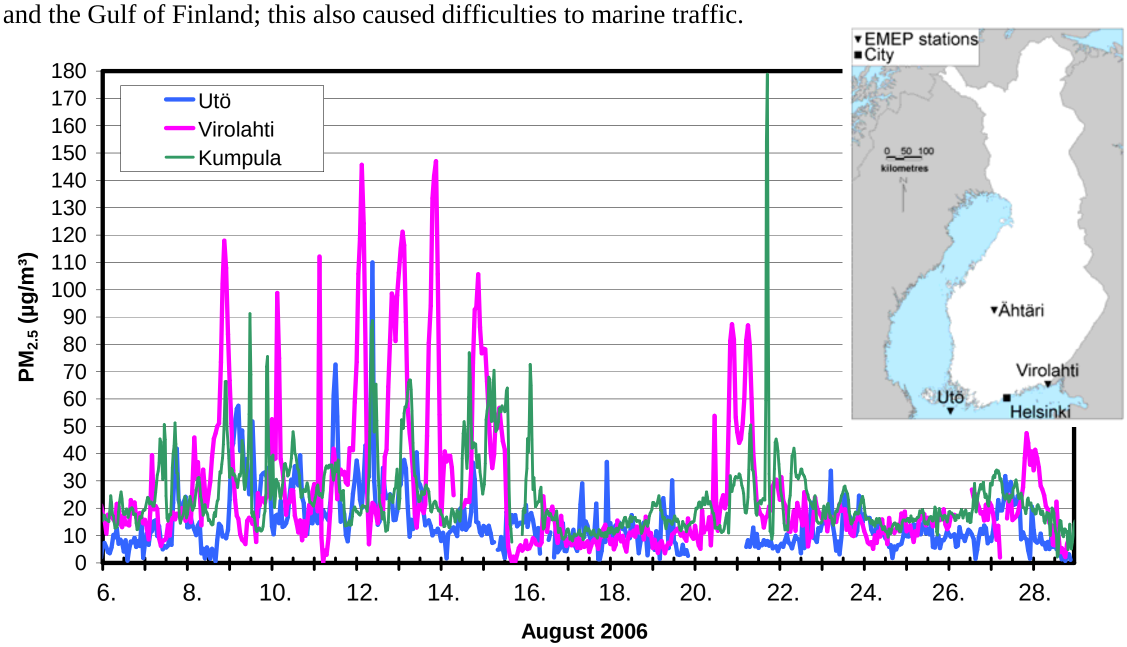

Figure 1. *The measured $PM_{2.5}$ concentrations at the urban background station of Kumpula in Helsinki, and at the regional background stations of Utö and Virolahti in Southern Finland from 6 to 28 of August, 2006.*

2.3 Dispersion modelling by the SILAM model

The air quality modelling system SILAM (e.g., Sofiev et al., 2006) was used for forecasting of the $PM_{2.5}$ concentrations originated from biomass burning (http://silam.fmi.fi). The forecasting system utilizes as input data near real-time satellite-based information on fires, and meteorological data from either the HIRLAM or ECMWF numerical weather prediction models. The emission fluxes of $PM_{2.5}$ from wildland fires were evaluated based on the daily averaged MODIS temperature anomalies (TA). We also applied a normalization function that describes the hourly diurnal variation of the fire intensity. The emission flux is equal to the product of a constant emission factor, TA and the diurnal normalization function. The final emission dataset consists of sequential hourly $PM_{2.5}$ emission fluxes, aggregated to a spatial resolution of 20 km. The model for evaluating the emissions based on the MODIS data has described in more detail by Saarikoski et al. (2007).

3. RESULTS AND DISCUSSION

The fine particulate matter observed at the station of Kumpula during the episode in August of 2006 consisted mainly of organic carbon (ca. 70%), while soot (black carbon) concentrations where low (Saarikoski et al., 2006).

This is an indication of smouldering fire, and may have implications on the initial plume height, which is higher for flaming fires due to higher temperatures.

During the episode in the Helsinki Metropolitan area in August of 2006, the high concentration peaks were temporally shorter, compared with those during the previous major wildland fire episodes in spring of 2006 (the latter have been discussed in detail by Saarikoski et al., (2007)). This was caused by the vicinity of the fire areas for the episodes in August; for the episodes in spring, the fire areas were located at the distances of hundreds or even more than a thousand kilometres from Helsinki. On August 21, weather in the Helsinki Metropolitan area was cloudy, but precipitation rates were low. Some light rain showers occurred in the morning and later in the night (Fig 2). Wind speed increased in the afternoon and wind was mainly south-easterly. During August 21, the nighttime mixing height based on ceilometer observations was between 200 and 300 m, while the daytime mixing height was about 500 meters (Fig 2). The pollutant episodes can be distinguished from normal situations because of a very strong ceilometer backscattering. The ceilometer, however, does not distinguish a particulate matter episode from a rain or a fog, so the final assessment of the reason for the strong backscatter has to be based on other supplementary measurements.

a) b)

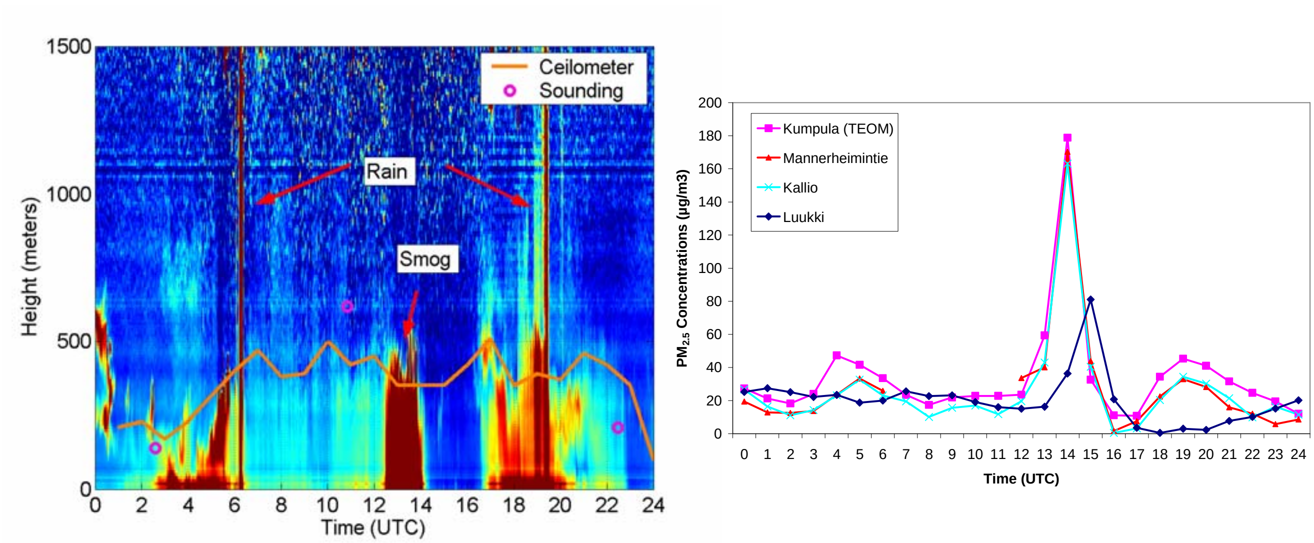

Figure 2. *a) 24-h period of ceilometer echo intensity observations at Vallila, Helsinki, 21 August 2006. The height of the MH determined by the ceilometer and radiosoundings are superimposed on the ceilometer raw echo data. b) 24-h period of $PM_{2.5}$ concentrations in Helsinki Metropolitan area, 21 August 2006.*

In Helsinki metropolitan area, the wind speed increased in the afternoon of 21 August, 2006, and the wind direction was mainly between easterly and south-easterly. In the late afternoon, wind direction temporarily changed between north and east. In the evening, the wind direction returned to between east and southeast and the wind speed decreased.

The SILAM model forecasted well the timing of the occurrence of the highest $PM_{2.5}$ concentrations in Helsinki, as well as the overall temporal and spatial distribution of the concentration plumes; this can be shown by a detailed comparison of modelled and measured data (not shown here). However, the measured $PM_{2.5}$ concentrations in Helsinki were underpredicted by the model. Some example results have been presented in Fig. 3. Clearly, the accuracy of the dispersion modelling is limited by the resolutions of the meteorological data and the accuracy of the emission modelling.

4. CONCLUSIONS

The regionally transported smokes emitted by biomass burning had a strong impact on the $PM_{2.5}$ mass concentrations in Helsinki from 18 July to 28 August, 2006. During the episode in Helsinki, the high concentration peaks were temporally shorter, compared with those during the previous major wildland fire episodes in spring of 2006. This was caused by the closer vicinity of the fire areas for the episode in August. The fine particulate matter observed at the station of Kumpula during the episode consisted mainly of organic carbon (ca. 70%), while soot (black carbon) concentrations where low. This is an indication of smouldering fire.

We have also implemented a semi-operational forecasting system in case of wild-land fires; the results are publicly available at http://silam.fmi.fi. The SILAM model forecasted well the overall temporal and spatial distribution of the concentration plumes; however, the absolute values of the fine particular matter concentrations were underpredicted due to inaccuracies in the emission modelling. More research is needed especially regarding the evaluation of wildland fire emissions, based on satellite observations.

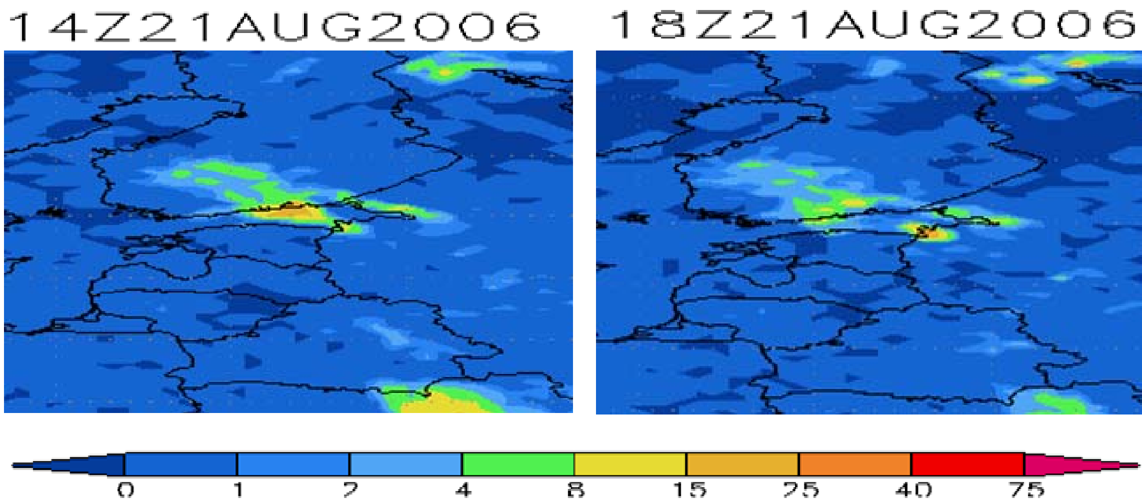

Figure 3. *The forecasted $PM_{2.5}$ concentrations ($\mu g/m^3$) using the SILAM model at 14 and 18 UTC on 21 August, 2006.*

6. REFERENCES

Holzworth, C. G., 1964: Estimates of mean maximum mixing depths in the contiguous United States. *Monthly Weather Review*, 92, 235-242.

Holzworth, C. G., 1967: Mixing depths, wind speeds and air pollution potential for selected locations in the United States. *Journal of Applied Meteorology*, 6, 1039-1044.

Joffre, S. M., Kangas, M., Heikinheimo, M. and Kitaigorodskii, S. A., 2001: Variability of the stable and unstable atmospheric boundary-layer height and its scales over a boreal forest. *Boundary-Layer Meterology*, 99, 429-450

Saarikoski, S., Sillanpää, M., Saarnio, K., Timonen, H., Teinilä, K. and Hillamo, R., 2006. Chemical composition of fine particles in major biomass burning episodes observed in Finland in 2006. In NOSA 2006 Aerosol symposium Helsinki 8.-10.11.2006 (Ed., Vehkamäki, Bergman, Julin, Salonen and Kulmala). Report series in Aerosol Science 83, 325-329.

Saarikoski, S., Sillanpää, M., Sofiev, M., Timonen, H., Saarnio, K., Teinilä, K., Karppinen, A., Kukkonen, J. and Hillamo, R., 2007. Major biomass burning episode in northern Europe in spring 2006: the chemical composition and atmospheric chemistry of aerosols. *Atmospheric Environment* (in print).

Sofiev M, Siljamo P, Valkama I, Ilvonen M and Kukkonen J., 2006: A dispersion modelling system SILAM and its evaluation against ETEX data. *Atmospheric Environment*; 40/4: 674-685.

Steyn, D. G., Baldi, M. and Hoff, R. M., 1999: The detection of mixed layer depth and entrainment zone thickness from lidar backscatter profiles. *Journal of Atmospheric and Oceanic Technology*, 16, 953-959.

PERFORMANCE OF MODELS-3/CMAQ FOR PREDICTING URBAN AND REGIONAL CONCENTRATIONS OF O_3 AND NO_2 DURING A SUMMER EPISODE IN THE SOUTHEAST OF ENGLAND, UK

Y Yu[1], N Kitwroon[1], R S Sokhi[1], D R Middleton[2] and B Fisher[3]
[1]Centre for Atmospheric and Instrumentation Research (CAIR), University of Hertfordshire, Hatfield, Hertfordshire, AL10 9AB, United Kingdom
[2]Met Office, FitzRoy Road, Exeter EX1 3PB, U.K, [3]Environment Agency, Reading, RG1 8DQ, U.K.

ABSTRACT

The Models3/CMQ was applied to a summer high ozone (O_3) and nitrogen dioxide (NO_2) episode occurred during 22-28 June 2001. Hourly mixing ratios of O_3 and NO_2.from model runs with two different horizontal grid spacing were compared with available observations. Qualitative and quantitative evaluations show that the model can capture the diurnal variations and spatial distributions of O_3 and NO_2 concentrations very well. On average, the model slightly under-predicts O_3 concentrations with a mean bias of –3.6µg m^{-3} and -0.8µg m^{-3} for the 3 km and 9 km resolution, respectively. This is largely due to the under-estimation of daytime peaks during high ozone days. Simulations for NO_2 tend to show much larger bias and error than the similar statistics for O_3. While the 9-km and the 3-km resolution simulations give comparable model performance for O_3, there is a tendency for the finer resolution simulation to give better statistic scores for NO_2 concentrations.

1. INTRODUCTION

Air quality monitoring, especially through coordinated networks, provides information on the extent of the pollution and exceedances of target and limit values. However air quality monitoring does not provide all the information required in the design of air quality strategies, for example, it does not help define the ways of meeting targets and to assess the effectiveness of control strategies. There has been an increased use of advanced air quality models, such as Models-3, in Europe (e.g. San Jose et al., 2007; Sokhi et al. 2006), North America (e.g. Smyth et al. 2006) and most recently in Asia (e.g. Chen et al. 2007) for both scientific studies and regulatory assessment. However, rather little numerical modelling work, using such type of models, has been conducted to simulate air pollutant concentrations within the UK. Traditionlly, dispersion models with simplified treatment for meteorology and chemistry have been adopted as policy tools in the UK. Recently, there is growing interest in investigating the potential of CMAQ for regulatory applications in the UK (e.g. Cocks et al, 2003). In order to assess its performance and to build confidence in its use by UK air quality regulators, it is important to develop a good understanding of CMAQ's ability to simulate concentrations of regulated pollutants. The purpose of the present study is to compare simulated near-surface hourly concentrations of O_3 and NO_2 with observations and to evaluate whether CMAQ can predict O_3 and NO_2 concentrations consistent with observations for the selected period. The evaluation focuses on a summer episode during June 2001 affecting the southeast of England, UK.

2. MODEL SETUP AND INPUTS

2.1 The modelling system

CMAQ version 4.4 was used in this study. A modified version of the CB-4 chemical mechanism (Gery et al. 1994), named 'cb4_ae3_aq', was used for the gas phase chemistry, along with the 'smvgear'' chemistry solver. The NCAR/PSU Fifth generation Mesoscale Model MM5 (Grell et al., 1994) was used to generate meteorological fields for CMAQ. Emissions were processed using Sparse Matrix Operator Kernel Emissions (SMOKE) system (CEP, 2003).

2.2 CMAQ modelling domain and simulation period

Four nested domains (see Fig.1) were configured with the innermost domain having a spatial resolution of 3 km. The outermost model domain has been set-up to be large enough to reduce the possible effect of model boundary conditions on the overall model predictions. Twenty-six vertical σ-levels extend from the surface to an altitude of about 14 km. Vertical layers were unevenly distributed with fifteen layers in the lowest kilometre. The model starts at 12:00GMT 22 Jun. 2001 and ends at 12:00GMT 28 June 2001.

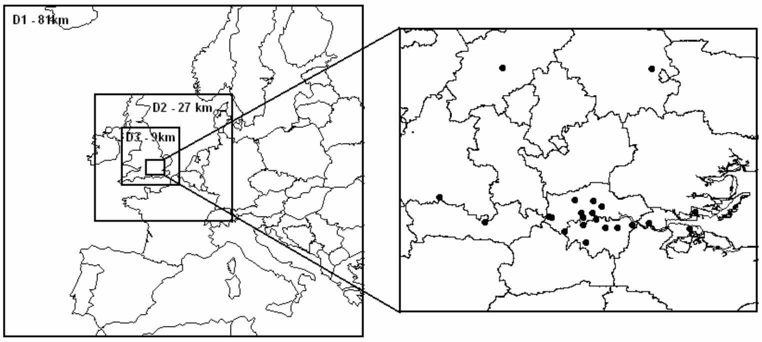

Figure 1. Left: The nested CMAQ modelling domain; right: the inner CMAQ domain and locations of air quality monitoring stations (black dots).

2.3 Model input preparation

The MM5 model was run with four two-way nested domains having the same grid resolutions as CMAQ. The physical options used in MM5 include Dudhia simple ice microphysics scheme, Grell cumulus scheme for the outer three domains (no cumulus scheme was used in the 3-km domain), MRF PBL scheme and 5-layer soil model. The ECMWF $1^{o}\times1^{o}$ reanalysis data available at every 6 h at the BADC were used to provide the boundary and initial condition for MM5.

The 50-km gridded annual anthropogenic emissions from the EMEP for year 2002 (http://webdab.emep.int/) were used for model grids outside of the UK. UK emissions for the nested 27, 9 and 3 km domains were taken from the National Atmospheric Emissions Inventory (NAEI) (http://www.naei.org.uk/), which holds 1 km resolution emissions data. Annual emissions and information on locations for point sources were extracted from the EPER (European Pollutant Emission Register) and NAEI. All the emissions data were reformatted and assigned country/state/county code before processing using SMOKE. Monthly, daily and hourly temporal profiles for the emissions were provide by the IER (Institute for Energy Economics and Rational Use of Energy, University of Stuttgart (private communication) and derived from Jenkin et al. (2000). Speciation profiles for NMVOCs were derived from the detailed UK VOC speciation given in Dore et al.(2004). Biogenic emissions of isoprene and monoterpenes were calculated following the method of Guenther et al. (1995).

The initial and boundary conditions for CMAQ for the coarsest domain were generated based on monthly mean data from the UK Meteorological Office global Lagrangian tropospheric 3-D chemical transport model (STOCHEM) (Derwent R 2006, personal communication). To reduce the effect of initial conditions, all the simulations are given a spin-up time of 48 hrs.

3. MODEL RESULTS

Measured hourly air quality data at 22 monitoring stations shown in Fig.1 (right) were used in the model evaluation for CMAQ. Qualitatively, the model simulates the diurnal O_3 and NO_2 concentration patterns very well at all sites. Fig. 2 compares the measured O_3 and NO_2 time series with the modelled results extracted from the first model level (about 14 m AGL) at two representative sites. At both sites, the model captures the O_3 night time lows quite well, but it tends to underpredict daytime peaks during high ozone days, for example on 24 June at London Bexley (urban background) and on 25 June and 26 June at Harwell (rural).

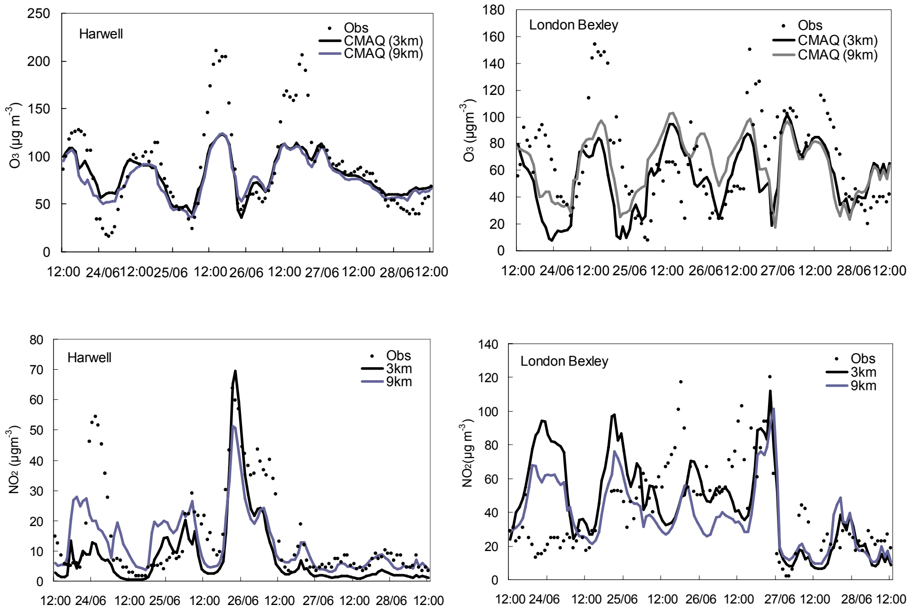

Figure 2 Comparison of measured and modelled time series of O_3 (upper two panels) and NO_2 (lower two panels) concentrations at London Bexley (urban background) and Harwell (rural).

Figure 3 shows scatter plots of measured–modelled O_3 (left panel) and NO_2 pairs (right panel) for all the modelling hours and sites for the 3-km resolution simulation. Table 1 summarizes the corresponding O_3 and NO_2 performance statistics for both 9-km and 3-km resolution simulations for the innermost domain.

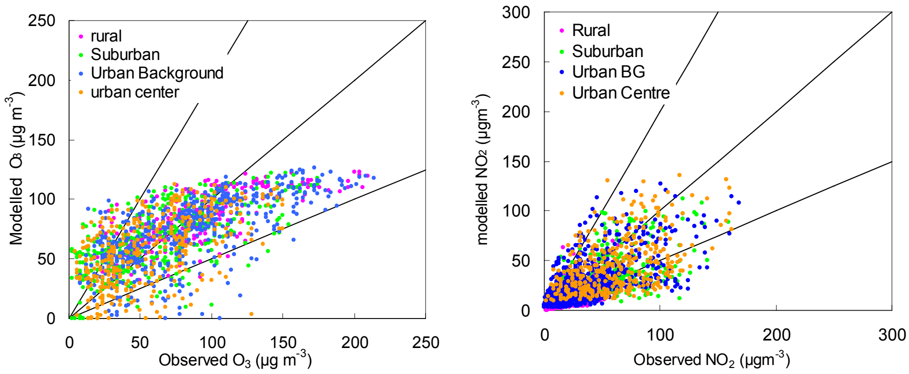

Figure 3 Measured versus modelled O_3 (left) and NO_2 (right) concentration for all data pairs. Modelled O_3 and NO_2 concentrations were extracted from the first model level (about 14 m AGL).

On average, the model slightly under-predicts O_3 concentrations with a mean bias (MB) of -3.6μg m^{-3} and -0.8μg m^{-3} for 3 km and 9 km resolution, respectively. In total, nearly 82% of all modelled concentrations are within a factor of 2 of the corresponding measured O_3 concentrations. The 9-km and the 3-km resolution simulations give comparable model performance for most of the observational sites but a better performance is achieved by the 3-km resolution simulation at sub-urban and urban centre sites, where the effects of local sources are more important.

Overall the model significantly under-predicts NO_2 concentrations with a MB of –22.5 μg m^{-3} and –25 μg m^{-3} for 3 km and 9 km resolution simulations, respectively. Over all the sites, nearly 60 % of modelled concentrations are within a factor of 2 of the corresponding measured values. In general the 3-km resolution gives better predictions than the 9-km resolution simulation, especially for urban areas.

Table 1. Quantitative performance statistics for near surface O_3 and NO_2 predictions for all stations within the 3-km domain, i.e. domain 4.

Statistics	O_3		NO_2	
	3km	9km	3km	9km
Mean Observation (μg m^{-3})	73.3	73.3	39.8	39.8
Mean Modelled (μg m^{-3})	69.6	72.4	28.0	25.3
Correlation Coefficient.	0.69	0.66	0.68	0.63
Mean Bias (MB) (μg m^{-3})	-3.6	-0.8	-11.8	-14.5
Mean Normalized Bias (MNB) %	30.4	39.4	-10.5	-12.8
Mean Error (ME) (μg m^{-3})	24.2	25.2	18.3	20.1
Mean Normalized Error (MNE) %	59.8	69.9	54.4	60.6
Root Mean Square Error (RMSE) (μg m^{-3})	31.2	31.9	25.9	28.4

4. CONCLUSIONS

The CMAQ model was able to reproduce the observed temporal and spatial variations of O_3 and NO_2. Model performance was better for O_3 than for NO_2. Statistical parameters indicate a satisfactory overall model performance. However the model tends to miss very high peak O_3 values. The cause of this disagreement is under investigation as part of a wider programme of research on comparison and application of regional models in the UK. For O_3 the 9-km and the 3-km resolution simulations gave comparable model performance. For NO_2, generally the 3-km resolution gives better predictions than the 9-km resolution simulation.

ACKNOWLEDGEMENT

This work is supported by the UK Environment Agency and the Air4EU project funded under FP6. AIR4EU is a member project of the Cluster of European Air Quality Research (CLEAR).

REFERENCES

San Jose, R., Perez, J.L., Gonzalez, R.M., 2007. An operational real-time air quality modelling system for industrial plants. Environmental Modelling & Software 22, 297-307.

Sokhi, R.S., Jose, R.S., Kitwiroon, N., Fragkou, E., Perez, J.L., Middleton, D.R., 2006. Prediction of ozone levels in London using the MM5-CMAQ modelling system. Environmental Modelling & Software 21, 566-576.

Chen, D.S. et al.2007. An integrated MM5-CMAQ modeling approach for assessing trans-boundary PM10 contribution to the host city of 2008 Olympic Summer Games e Beijing, China. Atmospheric Environment 41, 1237-1250.

Smyth, S.C., Jiang, W., Yin, D., Roth, H., Giroux, E.,2006, Evaluation of CMAQ O3 and PM2.5 performance using Pacific 2001 measurement data. Atmospheric Environment 40, 2735–2749.

Cocks A.T., Lucas V., Rodgers I.R., Teasdale I., 2003. The performance of Models 3 for deposition and atmospheric concentrations over a year. R&D Technical Report, RWE Innogy Environment.

Gerry, M.W., Whitten, G.Z., Killus, J. P., Dodge, M. C., 1994 A photochemical kinetic mechanism for urban and regional scale computer modeling. Journal of Geophysical Research 94, 12925–12956.

Grell, G. A., Dudhia, J., Stauffer, D.R., 1994, A description of the Fifth-Generation Penn State/NCAR Mesoscale Model (MM5). NCAR Technical Note, NCAR/TN-398+STR, National Center for Atmospheric Research, Boulder, CO.

CEP, 2003 Sparse Matrix Operator Kernel Emission (SMOKE) modeling system, University of North Carolina, Carolina Environmental Programs, Chapel Hill, NC.

Jenkin M E, Murrells T P, and Passant N R, 2000 The temporal dependence of ozone precursor emissions: estimation and application, AEAT/R/ENV/0355, AEA Technology, Harwell.

Dore C J, Watterson J D, Goodwin J W L, et al., 2004 UK Emissions of Air Pollutants 1970 to 2002, AEA Technology.

Guenther A, Hewitt C N, Erickson D, et al., 1995 A global model of natural volatile organic compound emissions. Journal of Geophysical Research, 100 (D5), 8873-8892.

EVALUATION OF THE INFLUENCE OF WILD LAND FIRES ON AIR QUALITY IN CITIES – COMBINED UTILISATION OF GROUND- AND SATELLITE-BASED OBSERVATIONS AND MODELLING

Jaakko Kukkonen; Sanna Saarikoski; Markus Sillanpää; Hilkka Timonen; Karri Saarnio; Kimmo Teinilä; Mikhail Sofiev; Ari Karppinen; Risto Hillamo
Finnish Meteorological Institute

ABSTRACT

This paper evaluates the capabilities and limitations of currently available methodologies for the analysis of plumes originated from wildland fires. The $PM_{2.5}$ concentrations originated from biomass burning can be distinguished using ground-based measurements by the determination of tracer substances, such as, levoglucosan, potassium and oxalate; the concentrations of which are substantially increased during wildland fires. Both fire areas and smoke plumes can be detected from satellites using, e.g., the MODIS instrument. The emissions of $PM_{2.5}$ can be evaluated based on the satellite-detected temperature anomalies, and used as input data for regional and continental -scale dispersion models. The main uncertainties of the modelling methods are related to the evaluation of the emissions and their initial buoyancy based on satellite-based information, and the influence of the cloud cover on satellite measurements. The models have also not been sufficiently compared with either experimental ground- or satellite-based data up to date.

1. INTRODUCTION

Land and forest fires (collectively referred to as wildland fires) have serious negative impacts on human safety, air quality and health, regional and global climate change and regional economies (e.g., tourism, transport, aircraft operations). Forest fires can substantially increase the regional scale emissions of greenhouse gases and particulate matter into the atmosphere, especially during spring and summer.

The smoke from biomass burning contains numerous gaseous (e.g., CO and VOC's) and particulate compounds (e.g., PAH's and other organics) that are known to be hazardous to human health. Fire plumes can be transported all over Europe, where they can constitute a serious health risk for the population. For quantitative information of the effects of wildland fires, accurate estimates are needed (i) on the size of the burning area, (ii) the fire intensity and initial elevation of the plume, (iii) the emissions of particulate matter and gaseous pollutants, (iv) the transport and evolution of the resulting pollutant plume.

The objective of this paper is to evaluate the advantages and limitations of the currently available methodologies for the analysis of plumes originated from wild land fires. The potential of the currently available methods used at the Finnish Meteorological Institute is illustrated by presenting an analysis of an exceptionally severe and wide-spread biomass burning episode in Northern Europe in spring 2006. This episode has been previously analysed in detail by the present authors (Saarikoski et al., 2006, 2007). The transport of the smoke originated from these wild-land fires has also been previously studied using the FLEXPART particle dispersion model, together with the MODIS retrievals of the aerosol optical depth and AIRS retrievals of carbon monoxide (CO) total columns by Stohl et al. (2006).

This paper is associated to the paper by Rantamäki et al. (2007, these proceedings), which presents an analysis of another wildland fire episode that occurred in August 2006.

2. MATERIALS AND METHODS

We have developed a semi-operational, nearly real-time assessment system for forest fires that contains the following information and tools (clearly, some parts are available from third parties):

1. a pre-processing module that uses the forest fire observations of the MODIS satellite instrument (http://rapidfire.sci.gsfc.nasa.gov/subsets/),
2. modelling of the emissions and atmospheric dispersion of $PM_{2.5}$ from forest fires (http://silam.fmi.fi/),
3. the monitoring of the concentrations of $PM_{2.5}$ or PM_{10} at several air quality stations in Finland (http://www.fmi.fi/ilmanlaatu/ilatausta_20.html) and

4. the measurements of the chemical composition and specific wood burning tracer substances of particulate matter at one station.

The forecasts of the modelling system are publicly available at http://silam.fmi.fi.

2.1 Experimental methods

Part of the measurements of this study were performed in Helsinki, Finland, at an urban background station SMEAR III (60°20'N, 24°97'E, 26 m above sea level, for more details see http://www.atm.helsinki.fi/SMEAR/). Real-time measurements were done with a Twin-TEOM for $PM_{2.5}$ and $PM_{2.5-10}$, a PILS-IC for common ions and an aethalometer for black carbon. The 24-h PM_1 filter samples were analysed by using a thermal optical carbon analyser (elemental and organic carbon), a total carbon analyzer (watersoluble organic carbon), an ion chromatography (common ions) and a liquid chromatography mass spectrometer (levoglucosan).

2.2 Modelling

The air quality modeling system SILAM (e.g., Sofiev et al., 2006) was used for forecasting of the $PM_{2.5}$ concentrations originated from biomass burning (http://silam.fmi.fi). The forecasting system utilizes as input data near real-time satellite-based information on fires, and meteorological data from either the HIRLAM or ECMWF numerical weather prediction models.

The emission fluxes of $PM_{2.5}$ from wildland fires were evaluated based on the daily averaged MODIS temperature anomalies (TA). We utilized the procedures similar to those of GFEDv2 (Giglio et al., 2006), with a few amendments. We also applied a normalization function that describes the hourly diurnal variation of the fire intensity. The emission flux is equal to the product of a constant emission factor, TA and the diurnal normalization function. The final emission dataset consists of sequential hourly $PM_{2.5}$ emission fluxes, aggregated to a spatial resolution of 20 km. The model for evaluating the emissions based on the MODIS data has been described in more detail by Saarikoski et al. (2007).

3. RESULTS AND DISCUSSION

The measured concentrations of fine particular matter at Kumpula in spring of 2006 are presented in Figure 1.

The ground-based measurements provided the exact arrival and departure times of the smoke plumes in Helsinki. The long-range transported smokes had a strong impact on the $PM_{2.5}$ concentrations in Helsinki over the 12 days period in April and May, 2006. The $PM_{2.5}$ mass concentrations of biomass burning tracers - levoglucosan, potassium and oxalate - increased substantially during the first phases of the episode (from April 25 to May 5). The major portion of fine particle mass during the episodic periods was found to be organic carbon. The analyzed components allow a construction of the chemical mass closure of PM_1.

A dispersion model SILAM, coupled with the numerical weather prediction model HIRLAM, was used for the forecast of the $PM_{2.5}$ concentrations generated by biomass burning. According to the results of the MODIS satellite instrument and model simulations, the fire plumes were originated from wild land fires that were mainly situated in Western Russia. The hourly temporal variation of the measured and modelled concentrations agreed well during the duration of the episode, except during April 25-29, due to dense frontal clouds that prevented the detection of wild land fires by the MODIS instrument.

4. CONCLUSIONS

The SILAM model forecasted well the overall temporal and spatial distribution of the concentration plumes; however, the absolute values of the fine particular matter concentrations were underpredicted, due to inaccuracies in the emission modelling. The $PM_{2.5}$ concentrations originated from biomass burning can be distinguished using ground-based measurements by the determination of tracer substances, such as, levoglucosan, potassium and oxalate, and by determining the chemical composition of the fine particular matter, especially the concentration of organic carbon (Saarikoski et al., 2006, 2007).

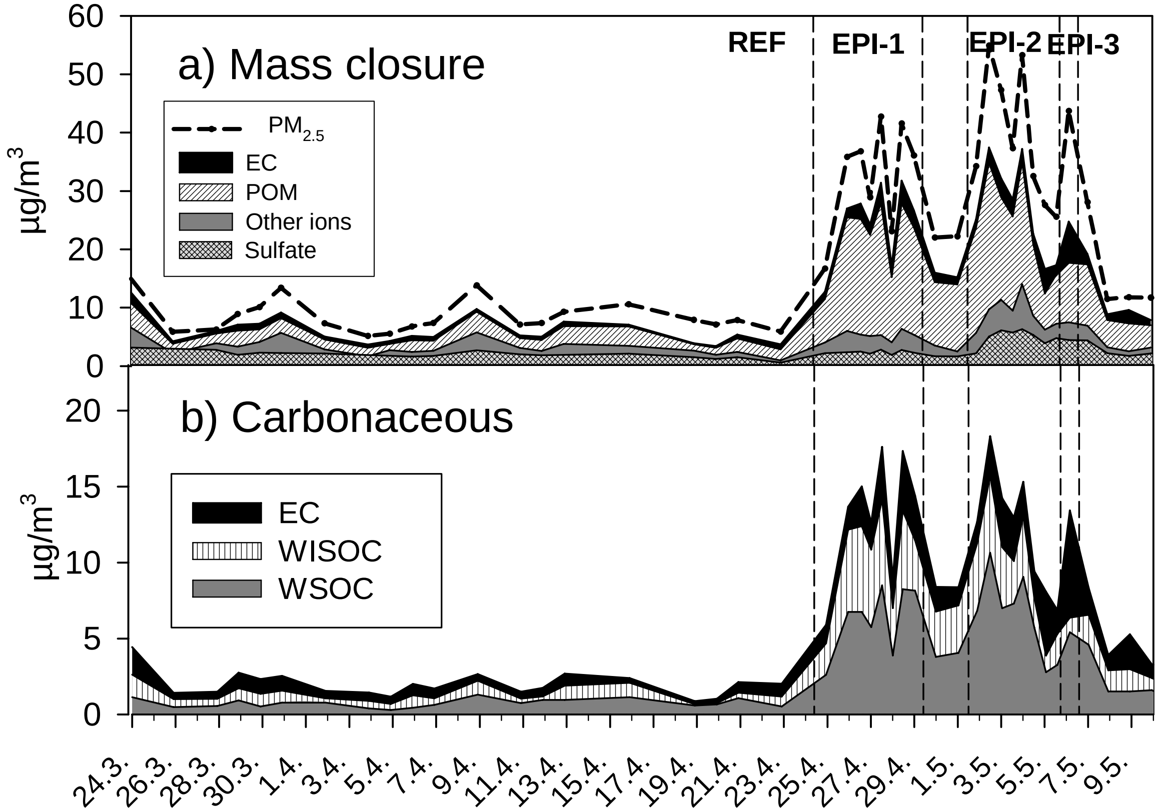

Figure 1. Mass closure for fine particles (a) and the composition of its carbonaceous fraction (b) prior and during the wildland fire episodes in Helsinki. $PM_{2.5}$ was measured with the TEOM whereas all the chemical components were analyzed from the PM_1 filters. REF, EPI-1, EPI-2 and EPI-3 stand for the reference period and three various episodes (Saarikoski et al., 2007).

More research is needed regarding the refinement and evaluation of satellite-based measurement techniques, especially on the detection of temperatures, types of fires (e.g., smouldering), and the formation of the source terms from fires. The initial buoyancy of the plume may have a substantial effect on the subsequent atmospheric dispersion. The models for the evaluation of wildland fire emissions, based on satellite observations, need evaluation against ground-based measurement campaigns and controlled experiments. The chemical and physical composition of the fire plumes formed in various conditions should be evaluated more extensively.

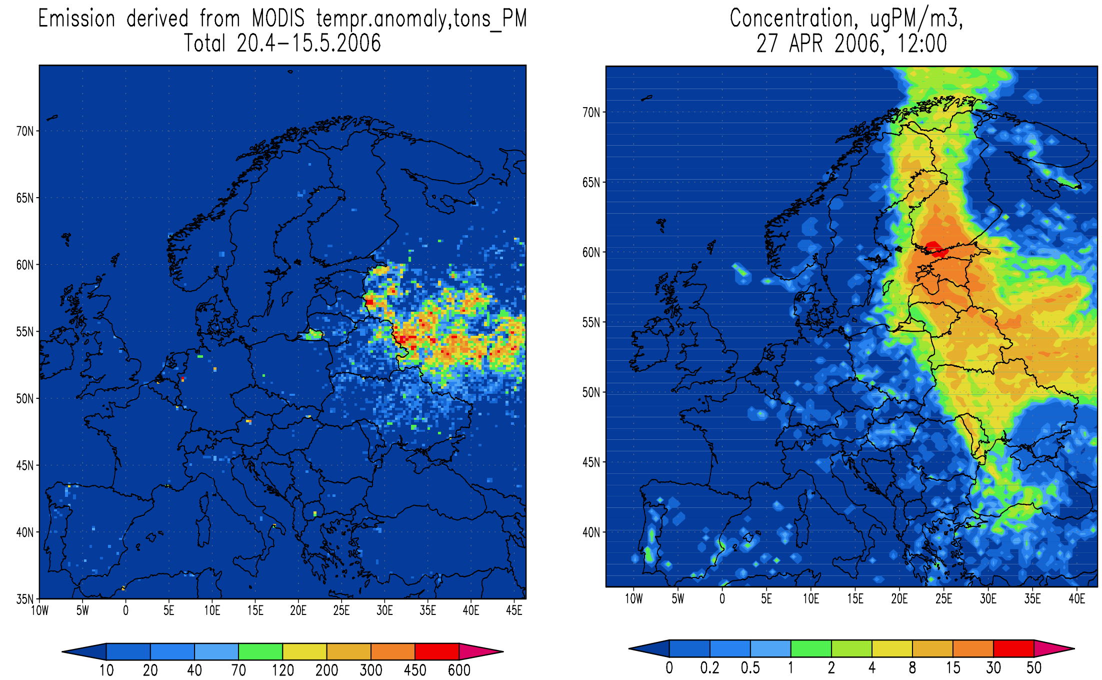

Figure 5. The mean predicted $PM_{2.5}$ emission flux originated from fires during April 20 – May 15, 2006, computed based on the measured MODIS temperature anomalies (left-hand panel, unit: tons PM), and $PM_{2.5}$ concentrations over Europe at 12:00 (UTC) April 27, 2006 (right-hand panel, unit: $\mu g/m^3$) (Saarikoski et al., 2007).

6. REFERENCES

Giglio, L., G.R. van der Werf, J.T. Randerson, G.J. Collatz,, P.S. Kasibhatla (2006). Global Estimation of Burned Area using MODIS Active Fire Observations, Atmospheric Chemistry and Physics, 6, 957-974. SRef-ID: 1680-7324/acp/2006-6-957.

Rantamäki, M., M. Sofiev, N. Eresmaa, S. Saarikoski, T. Mäkelä, R. Hillamo, A. Sarkanen, J. Kukkonen and A. Karppinen, 2007. EVALUATION OF A SEVERE AIR QUALITY EPISODE IN HELSINKI IN AUGUST 2006, CAUSED BY LONG-RANGE TRANSPORTED SMOKE. These proceedings.

Saarikoski, S., Sillanpää, M., Saarnio, K., Timonen, H., Teinilä, K. and Hillamo, R. (2006). Chemical composition of fine particles in major biomass burning episodes observed in Finland in 2006. In NOSA 2006 Aerosol symposium Helsinki 8.-10.11.2006 (Ed., Vehkamäki, Bergman, Julin, Salonen,and Kulmala). Report series in Aerosol Science 83, 325-329.

Saarikoski, S., Sillanpää, M., Sofiev, M., Timonen, H., Saarnio, K., Teinilä, K., Karppinen, A., Kukkonen, J. and Hillamo, R., 2007. Major biomass burning episode in northern Europe in spring 2006: the chemical composition and atmospheric chemistry of aerosols. Atmos.Environ. (in print).

Sofiev M, Siljamo P, Valkama I, Ilvonen M, Kukkonen J., 2006: A dispersion modelling system SILAM and its evaluation against ETEX data. Atmospheric Environment; 40/4: 674-685.

Stohl, A., T. Berg, J. F. Burkhart, A. M. Fjæraa, C. Forster, A. Herber, Ø. Hov, C. Lunder, W. W. McMillan, S. Oltmans, M. Shiobara, D. Simpson, S. Solberg, K. Stebel, J. Ström, K. Tørseth, R. Treffeisen, K. Virkkunen and K. E. Yttri, 2006. Arctic smoke – record high air pollution levels in the European Arctic due to agricultural fires in Eastern Europe. Atmos. Chem. Phys. Discuss., 6, 9655–9722.

Accounting for small-scale emission and concentration variability in air quality models

S. Galmarini[1], J.-F. Vinuesa[1] and A. Martilli[2]

[1]Institute for Environment and Sustainability
European Commission, DG-Joint Research Centre
TP 441, 21020 Ispra - Varese (Italy)

[2] CIEMAT, Madrid, Spain.

ABSTRACT
Urban and con-urban environments are characterized by heterogeneous emission that do not reflect in emission inventories if not as an average value and are not accounted for in meso- to limited area air quality model. The emissions are averaged over the grid cell where the emission source is located. The source can be linear (e.g. roads), surface (fields or urban areas) or punctual (factory) but after the averaging procedure, it is considered as a surface source with the same extension as the grid cell. This means that not only surface heterogeneity is lost in terms of its level of variability but also it will not be accounted for in the upper atmospheric levels and the impact of spatial distribution of emissions on spatial distribution of concentration is lost. This can represent a serious issue in case of passive as well as chemically reactive species or for the estimation of long or short term exposures. In this paper, we propose a novel approach to the problem including a formulation for the sub-grid variability of pollutant concentrations that takes into account the spatial heterogeneity of the emissions. The formulation that can be used in mesoscale models relies on the resolution of a prognostic equation for the sub-grid concentration variance, i.e. the quantity that accounts for the distribution of concentration within a grid-cell of a mesoscale model, by using a one-and-a-half order closure. The parameterization is implemented in a 1D column model and tested against large eddy simulations of convective atmospheric boundary layers.

1. INTRODUCTION

Accounting for sub-grid spatial variability of emission is still an open issue in atmospheric dispersion and in particular air quality modeling. The problem could be stated in these terms: how could one account for the fact that within a 3 to 10 Km (if not larger) resolution model, sources are sparsely distributed and emit variable quantities of mass to the atmosphere thus producing large sub-grid variability. To our knowledge this issue has never been tackled in the past. The typo of approach we have given to the problem solution relies on two different modeling tools.

2. METHODOLOGY AND RESULTS

A one-dimensional (1D) model and a Large-eddy simulation (LES) model are used with to different scopes, the first will host the parameterization developed to account for the process the second will generate all the control runs used to test the parameterization. The LES used here is the one developed by (Cuypers and Duynkerke, 1993). The one-dimensional model stems from the FVM model developed by (Martilli et al., 2002). The use of a LES with periodic boundary conditions coincides to the assumption of horizontal homogeneity that is the very same assumption adopted for a 1D model. When the three-dimensional results of a LES are averaged according to the x and y directions and time they can be reduced to a vertical profile that coincides with a 1D model. A preliminary comparison of the 1D model results and the LES is given in Figure 1. They relate to temperature, U and V components of the wind. The case simulated is a 2 h steady state convective boundary layer with a synoptic wind of 10 m/s. The LES results relate to and average over the last hour. The two models, not surprisingly compare very well. Having demonstrated that our assumptions are correct we can now formulate the problem concerning emissions and present our solution.
Let us assume that within a grid cell of 12x12 km^2 (coinciding with the LES domain size with a resolution of 100m x 100m) we have a source with finite dimensions. More specifically we will consider the case of a surface that is 1/4 of the grid cell and 1/20 of it. The normal practice would be to average the emission from the source over the grid cell size and to use it as source term to solve the average concentration equation in order to account for the atmospheric dispersion in the vertical (in a 1D model).

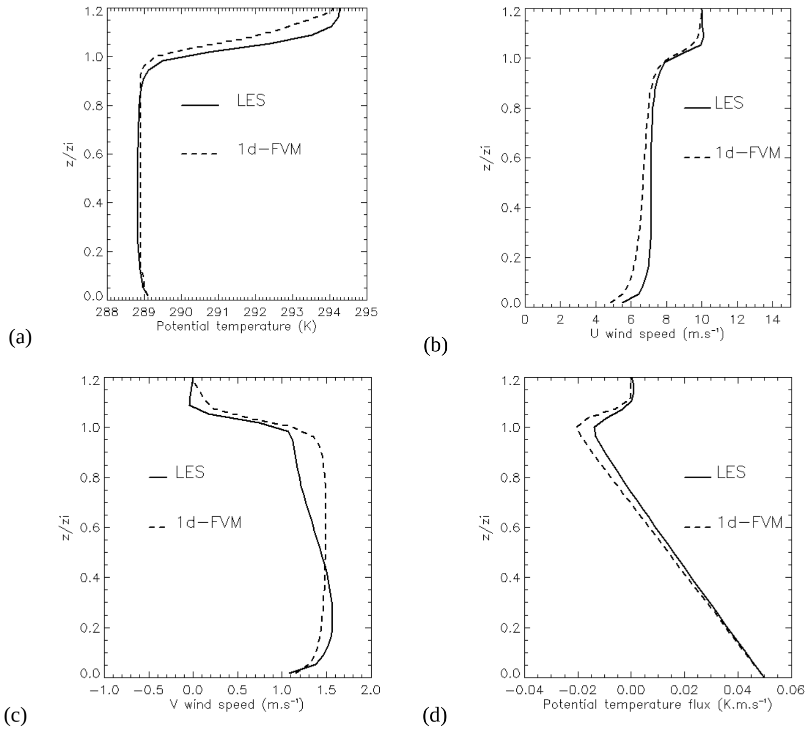

Figure 1: Comparison of LES results with the 1D model for (a) Potential temperature, (b and c) U and V component of the wind, (d) turbulent temperature flux.

This is what we have done with our 1D model and in Figure 2a the comparison with the LES is produced. The two models agree even on the mean concentration calculation. In Figure 2a you can see the two LES results for the two sources whereas those of the 1D coincide. The assumption is in fact that the two sources have different surface dimensions but emit the same amount of mass.

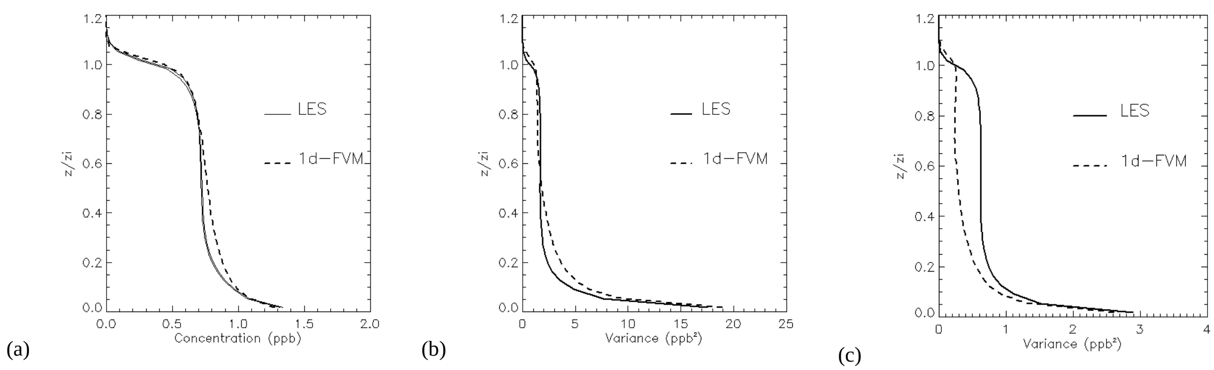

Figure 2: Comparison of LES results with the 1D model for (a) Concentration the two continuous lines correspond to the two emission scenarios (see text), (b) concentration variance emission scenario 0.05 Emission Surface/Grid Cell, (c) concentration variance emission scenario 0.25 Emission Surface/Grid Cell.

However the question remains: Does this result account for the fact that in the case of the first source only 1/4 of the surface and 1/20 of the second were respectively effectively emitting? Should not one transport also the variability in space together with the mean concentration? How can we account for that?

We propose here a parameterization to account for this variability that is based the conservation equation of the concentration variance. The latter reads:

$$\frac{\partial \overline{c'^2}}{\partial t} + \bar{u}_j \frac{\partial \overline{c'^2}}{\partial x_j} = -2\overline{u_j' c'} \frac{\partial \bar{c}}{\partial x_j} + \frac{\partial \overline{u_j' c'^2}}{\partial x_j} + 2\epsilon_c \qquad (1)$$

And accounts for the time evolution of concentration variance (term 1 lhs) created by turbulent motion (term 2 rhs) and transported in the three dimensional (terms 2 lhs and rhs) space while it is dissipated (term 3 rhs). The 1-dimensional version of eq (1) reads:

$$\frac{\partial \overline{c'^2}}{\partial t} = -2\overline{w'c'} \frac{\partial \bar{c}}{\partial z} + \frac{\partial \overline{w'c'^2}}{\partial z} + 2\overline{c'E'} + 2\epsilon_c \qquad (2)$$

Equation 2 contains an extra term that accounts for the contribution to the variance production originating from the surface spatial variability of the emissions. In order to solve equation 2 for the variance we need to close some of the terms. While terms 1, 2 and 4 on the rhs can be closed by very conventionally and well assessed parameterizations for term 3 we propose the following:

$$\overline{c'E'} = r\left(\overline{E'^2}\right)^{1/2}\left(\overline{c'^2}\right)^{1/2} \qquad (3)$$

Were *r* is to be assumed as the correlation coefficient between the concentration and the emission variances.
We have deduced the r parameter from the LES simulation while the concentration variance can be calculated straight forwardly. Figure 2b and c show the result of the comparison between the LES variance and the 1D model variance for the 0.05 Emission Surface/Grid-Cell Surface (2b) and 0.25 Emission Surface/Grid-Cell Surface (2c).
From the beginning of this experiment we assumed that the LES was representing the real atmospheric motion due to the high resolution and accuracy in simulation atmospheric flow and dispersion. Within the LES domain we introduced four virtual measuring locations shown in Figure 3. In the same picture the two ground plumes generated by the two emission patterns can be distinguished (violet and blue contours). The contours show clearly the squared shape of the emission pattern and its advection to the right that comes back in through the left boundary due to the boundary conditions assumption.
What we want to investigate is how is the use of the emission variance parameterization going to improve the result of a 1D model when compared with instantaneous measurements collected at the four points 1-4 in Figure 3.

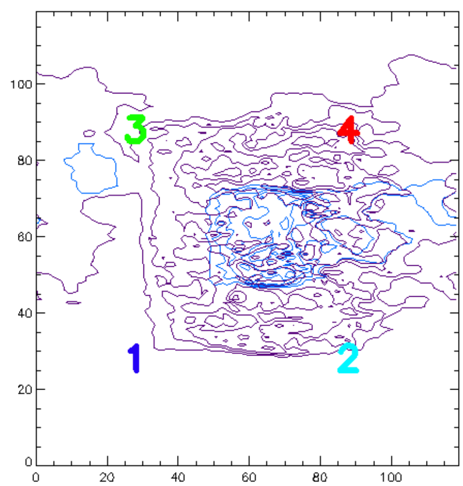

Figure 3: A snap shot of the LES simulation of the two emission patterns. Violet 0.25 Emission Surface/Grid-Cell Surface, blue 0.05 Emission Surface/Grid-Cell Surface. The numbers 1 trough 4 show the position of four virtual sampling locations were time profile of the concentrations for the two cases have been extracted.

The results are shown in Figures 4 (a-d). The figures show the time evolution of concentration sampled at two heights (12.5 m (a) and (b); 37.5 m (c) and (d)) for the two emission patterns ((a) and (c) 0.5 Emission Surface/Grid-Cell Surface; (b) and (d) same 0.25 Emission Surface/Grid-Cell Surface) at the four locations. The data are instantaneous concentration values produced by the LES with a 5 minutes frequency. The Thick black line are the concentrations obtained from the 1D model whereas the shading is correspond to + and – one standard deviation (the values below 0 have been discard as meaningless). As one can see the 1D model result can be better compared with the LES's in spite of the difference in modeling approaches. Even with the extreme case of comparing instantaneous equations with Reynolds Averaged ones, when we consider the spatial variability of the emissions we can manage to generalize the results of the 1D model.

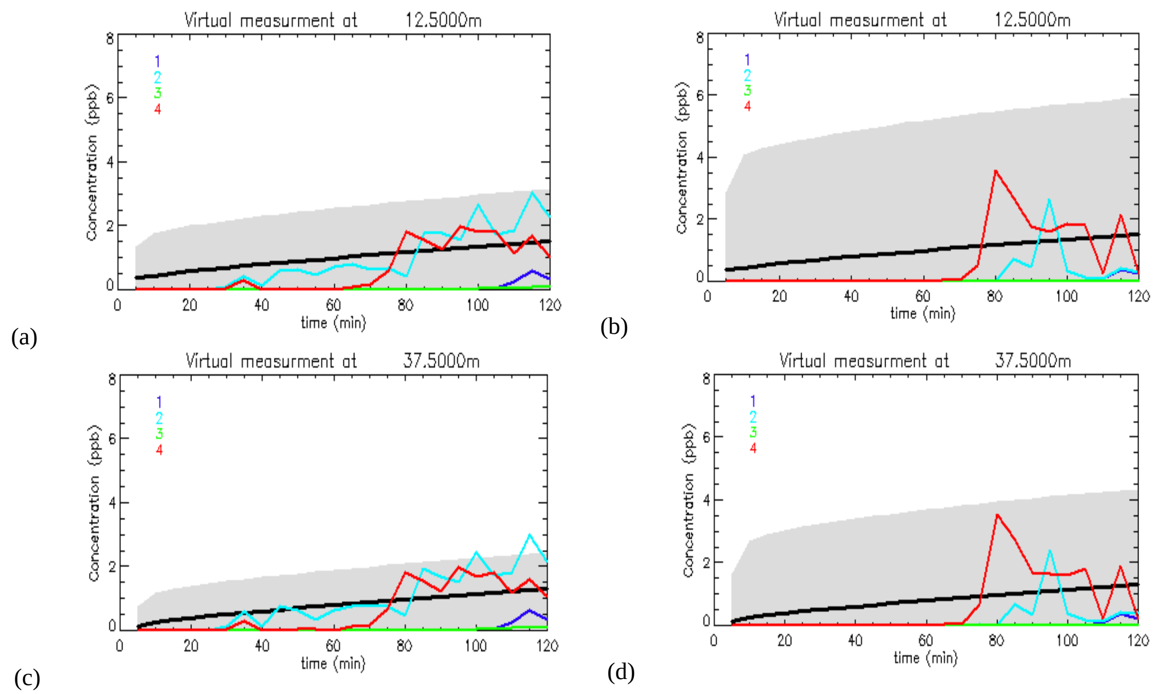

Figure 4: Time profile of the instantaneous concentrations sampled at the four locations given in Figure 3. The thick black line shows the average concentration obtained by the 1D model. The shading is the variance calculated with the new formulation. Panels (a) and (c) correspond to 0.05 Emission Surface/Grid-Cell Surface case sampling at 12.5 m and 37.5 respectively, panels (b) and (d) same as (a) and (b) but for the 0.25 Emission Surface/Grid-Cell Surface.

CONCLUSIONS

A new parameterization to account for inhomogeneous distribution of sub-grid emissions has been proposed. The results of the obtained with a 1D model compared to LES model are very encouraging. The next step will consider the analysis of different and more complex emission patterns and the development of a 3D version of the parameterization.

REFERENCES

Cuijpers, J.W. M., and Duynkerke P. G., 1993. Large eddy simulations of trade wind with cumulus clouds, J. Atmos. Sci. 50, 3894–3908

Martilli, A., 2002. Numerical study of urban impact on boundary layer structure: sensitivity to wind speed, urban morphology, and rural soil moisture. Journal of Applied Meteorology 41, 1247–1266.

BOUNDARY CONDITIONS AND THEIR IMPACT ON URBAN SCALE CTM SIMULATIONS

Douros I.[1], Naneris C.[1], Tsegas G.[1], Schaap M.[2] and Moussiopoulos N.[1]
[1] Aristotle University of Thessaloniki, Laboratory of Heat transfer and Environmental Engineering, Box 483, Aristotle University, Gr-54124, Thessaloniki, Greece
[2] TNO, Environmental Quality Department, P.O. Box 342, 7300 AH, Apeldoorn
The Netherlands

ABSTRACT
This work aims at identifying the sensitivity of Chemistry Transport Model (CTM) results on the choice of boundary conditions. It focuses both on initial and lateral boundary concentrations as well as the meteorological fields used to drive photochemical dispersion models. Furthermore, it evaluates quantitatively the relative impact of the aforementioned input on the simulated concentrations. The analysis has been performed by using OFIS, a Eulerian urban scale model capable of describing urban scale plume photochemistry and dispersion in a variety of situations. For the purposes of this analysis, boundary conditions coming from two different regional scale models systems (EMEP and LOTOS-EUROS) were used. Results show an equally significant effect of lateral boundary conditions and meteorology on the calculated concentrations, revealing the importance of using quality assured larger scale model results for feeding urban scale simulations, especially for pollutants such as NO_2 and O_3.
`

1. INTRODUCTION
The AIR4EU project aimed at developing recommendations to integrate measuring and modelling techniques into consistent, comprehensive and cost-effective air quality assessment methods (URL1). Within this project, a wide variety of factors that determine the air quality assessment process have been identified and evaluated. With regard to the use of modelling to assess air pollution at the urban/agglomerate scale, the quality assurance of input data was considered to be one of the most important aspects. In addition, effective formulation of control strategies for the ambient levels of various air pollutants requires knowledge of the sensitivity of the calculated concentrations of those pollutants not only to the primary and precursor emissions, but to every input data to the model, including initial and lateral boundary conditions.

As a means to circumvent or even overcome the substantial needs for boundary conditions, several CTMs (TAPM.v3, TM5 etc.) have gradually adopted even larger domains and a multiple nesting rationale in order to study the urban scale. Although this technique presents the advantage of a uniform approach to all the scales, it faces the shortcoming of high computational cost and is not always completely independent of boundary conditions. Typically, the study of the greater area of a European city requires a run for the whole of Europe which nests successive higher resolution runs that end up with an appropriate zoom in the city.

Most of urban scale CTMs in operational use today rely on boundary conditions from regional scale models. The objective of this study is to quantitatively evaluate the influence of boundary conditions using as a tool the Eulerian urban scale model OFIS. Rather than performing a sensitivity analysis in the classic way (i.e., investigating the model response to input data perturbations in order to evaluate the model behaviour), in the present study the CTM is assumed to be a reliable tool and different initial and boundary conditions are used in order to investigate their impact on the calculation results.

2. METHODOLOGY
One of the main aims for the development of the OFIS model was to provide a reliable tool for refining regional model simulations by estimating the urban subgrid effect on pollution levels (Arvanitis and Moussiopoulos, 2006, Moussiopoulos and Douros, 2004). OFIS simulates concentration changes due to the advection of species and chemical transformation in each cell of its computational domain, while the concentration values outside this domain are assumed to coincide with the regional background concentrations provided by the regional scale model. The model simulates separately each day of, typically, one year.

For the needs of the present study, the computational domain of the model consisted of a two-layer gridded strip with a length of 240 km and a width defined by the city size, with the city in the centre. For a specific time frame with a prevailing wind from NE, this domain setup is illustrated in Figure 1. The strip is oriented along the prevailing wind direction, altering direction when the meteorological input is modified (every 3 hours). The first vertical layer extended up to 90m (in accordance with the EMEP model), while the second one extended up to the mixing height, thus varying with time. The restriction to this computational domain results in a high computational speed and a low output file size. For prescribing the time evolution of both the mixing height and the turbulent exchange coefficient between the two layers, a 1D version of the non-hydrostatic meteorological model MEMO (Kunz and Moussiopoulos, 1997) is utilised. Emission data are inserted into the model in the form of gridded emission inventories. Emissions are calculated for each OFIS cell by properly taking into account the emission density of the underlying fine-scale inventory. Due to the modular structure of OFIS, chemical transformations can be treated by any suitable chemical reaction mechanism, the default being the EMEP MSC-W chemistry (Arvanitis and Moussiopoulos, 2003).

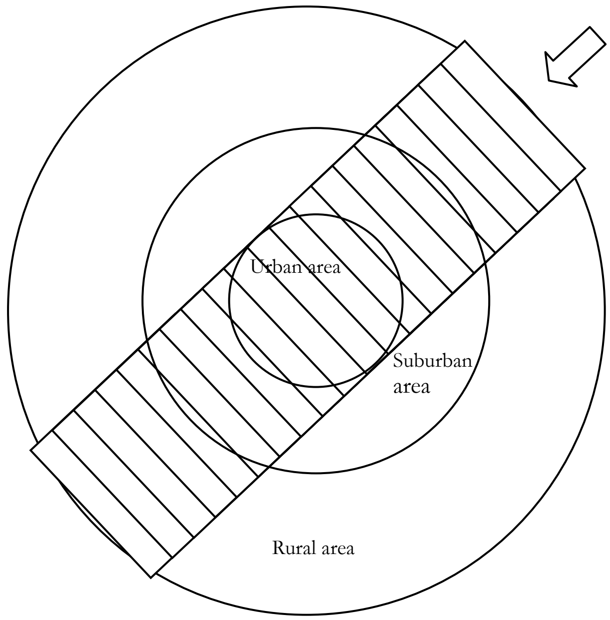

Figure 1. OFIS computational domain (gridded strip) and assumed geographic distribution of urban, suburban and rural areas.

Pollutant transport and transformation is calculated by solving the following equations for each grid cell of the computational domain and each species of the chemical mechanism in use:

$$\Delta c_i^1 / \Delta t = K_z (c_i^2 - c_i^1) / dz_1^{\,2} + q_i / dz_1 + R_i (c_1^1, \ldots, c_n^1) + u\,(c_i^{u1} - c_i^1) / \Delta \mathrm{x} \quad (1)$$

$$\Delta c_i^2 / \Delta t = K_z (c_i^1 - c_i^2) / (dz_2 dz_1) + R_i (c_1^2, \ldots, c_n^2) + u\,(c_i^{u2} - c_i^2) / \Delta \mathrm{x} + (c_i^{bc} - c_i^2) \max\left[0, \Delta H_t / (\Delta t \cdot H_t)\right] \quad (2)$$

where superscripts [1] and [2] refer to the two layers of the model, c_i is the concentration of chemical species i of the chemical mechanism, K_z is the vertical turbulent exchange coefficient, q_i is the emission rate for species I, R_i is the chemical formation or destruction rate for species i, Δx is the cell thickness along the wind direction, H_t is the mixing height, c_i^u is the upwind cell concentration of i and, c_i^{bc} is the concentration above the mixing height. R_i in the two equations is defined by the chemical mechanism in use, EMEP MSC-W for the purposes of this study. The numerical solution of the equation system is based on a variable step, second order BDF formula and a Gauss-Seidel iterative technique. Thus, the subject of this study is the response of the model to different values for the initial concentrations c_i for both layers, the lateral concentrations c_i^{u1}, c_i^{u2} and c_i^{bc}, as well as different meteorological input. Meteorological input is inserted into the model in the form of three variables, namely wind speed, direction and temperature (affecting R_i in the thermal chemical reactions, but also the calculation of H_t and K_z).

The EMEP Unified Model (URL2) which has been mostly used as a source of OFIS boundary conditions is an Eulerian grid model with European coverage, using a polar stereographic projection. The horizontal grid cell size of the model is 50×50 km^2, while in the vertical the model uses 20 layers, the first of which has a thickness of

approximately 90m. Meteorology for EMEP model runs originates from 3-hourly meteorological data from PARLAM-PS, a dedicated version of the HIRLAM (HIgh Resolution Limited Area Model) Numerical Weather Prediction (NWP) model (Sandnes and Tsyro, 2000). EMEP utilises various versions of the EMEP MSC-W chemical mechanism (Simpson, 1993).
LOTOS-EUROS (Schaap et al., 2005) is also a Eulerian grid model covering Europe with horizontal boundaries at 10ºW and 60ºE and at 35ºE and 70ºN. In horizontal direction the model domain is divided into 140×140 grid cells with a size of 0.5ºlon.×0.25ºlat. (~25×25 km^2). The lowest 3.5 km of the atmosphere are represented by three terrain following prognostic layers for which the continuity equation is solved and an additional (diagnostic) surface layer with a thickness of 25m. The LOTOS-EUROS system is presently driven by 3-hourly meteorological data produced by the Free University of Berlin employing a diagnostic meteorological analysis system based on an optimum interpolation procedure on isentropic surfaces (Kerschbaumer and Reimer, 2003), but also, meteorological data obtained from ECMWF can be used to force the model. The model uses a slightly adapted version of the CBM-IV chemical mechanism (Aldeman, 1999). This scheme contains 28 species and 66 reactions, including 12 photolytic reactions. Compared to the original scheme steady state approximations were used to reduce the number of reactions.

Several OFIS characteristics, especially its vertical structure, were selected to ensure an optimised application in conjunction with the EMEP model. This fact presented certain challenges in the formulation of boundary conditions data originating from a different regional model such as LOTOS-EUROS. More specifically, an appropriate mass-preserving interpolation scheme had to be applied to account for the different horizontal and vertical setup of the two regional models. In addition, a logarithmic law was applied in view of the different height at which wind speed was provided in each case. Finally, as the models use different chemical mechanisms, there was a need for a suitable correspondence between the chemical species available. Except for the cases where a straightforward one-to-one correspondence was possible (as in the cases of O_3, NO, NO_2, ethane, formaldehyde, xylene and various PM species), a split of the lumped CBM-IV alkanes, alkenes and aldehydes had to be performed in order to map them onto EMEP MSC-W species. This split was done following a statistical evaluation of the relative mixing ratios of the relevant EMEP MSC-W species in the output of the EMEP model.

For the purposes of the current investigation, the city of Athens was selected as a case study. The air quality in Athens for the year 2000 was analysed using measurements from seven urban background and suburban stations. In this way, the prevailing trends during this short time period have been revealed and they were then connected through the modelling study with the main contributing input data. Unfortunately no PM monitoring data were available for year 2000, and therefore this study was limited to gaseous species only.

3. RESULTS AND DISCUSSION

Three sets of runs were performed in order to identify how different boundary conditions affect the OFIS model results. The first two were by using the same source for boundary conditions (regarding concentrations) and meteorology, i.e. EMEP and LOTOS-EUROS respectively. As a means, however, to identify the importance of input meteorology, a third run was performed where concentration boundary conditions originated from LOTOS-EUROS, while meteorology was from EMEP (PARLAM-PS). The comparison between observed and modelled results for the mean annual values of NO_2 and O_3 is shown in figures 2 and 3. Table 1 provides the correlation coefficients for the three runs.

Table 1: Correlation coefficients for the mean annual modelled vs. observed NO_2 and O_3 concentrations at seven stations of the Greater Athens Area for the three runs

	EMEP BCs & MET	LOTOS BCs & MET	LOTOS BCs & EMEP MET
NO_2	0.64	0.51	0.66
O_3	0.35	0.23	0.57

It is evident that the runs differ substantially, most notably for O_3. This can be attributed to the steep gradient of O_3 concentrations in the first few layers of each regional model, a fact that renders OFIS very sensitive to the methodology that is used for the correspondence of vertical layers. Best results in terms of the correlation coefficient are achieved by the “mixed” run for both pollutants. The better performance of the “EMEP BCs and met” run compared to the “LOTOS BCs and met” run is not surprising if one considers the affinity of the EMEP and OFIS models, mostly reflected in the common treatment of vertical layers and chemistry.

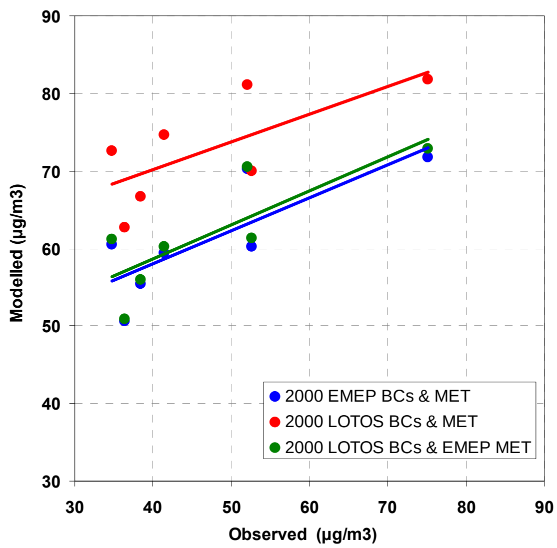

Figure 2: Scatter plot for annual mean NO_2 concentrations in Athens

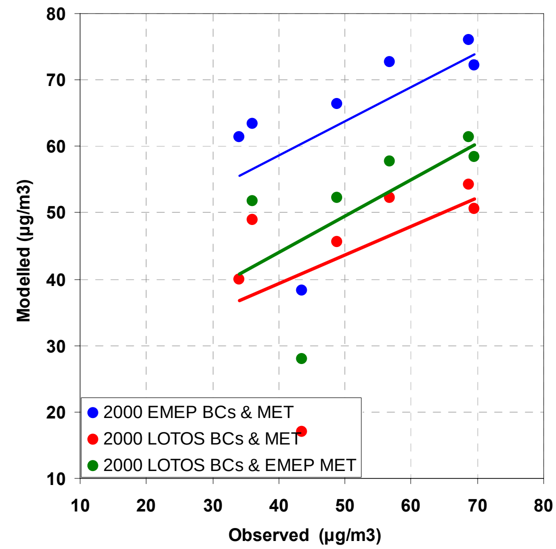

Figure 3: Scatter plot for annual mean O_3 concentrations in Athens

4. CONCLUSION

The AIR4EU project has attempted an in depth review of all aspects associated with the use of CTMs for air quality assessment purposes. The results of this work prove the importance of scale interactive processes, by indicating a significant dependence of urban scale model results on the input boundary conditions and meteorology from regional scale models. Except for the valuable information that these simulations have revealed about the sensitivity of the specific model, OFIS, they have most importantly proven the feasibility of comparative analyses with different available input data. In particular, the prospect of even better results with the use of concentration and meteorological fields from different regional models does not certainly comprise a proposed methodology, but rather enhances the notion that careful consideration and selection of all input parameters is crucial when applying CTMs, especially in the urban and local scales.

5. ACKNOWLEDGEMENTS

This work has been carried out within the framework of the AIR4EU project.

6. REFERENCES

Adelman, Z.E.1999. A re-evaluation of the Carbon Bond-IV photochemical mechanism. M.Sc. thesis, Department of Environmental Sciences and Engineering, School of Public Health, University of North Carolina, USA

Arvanitis A. and Moussiopoulos N. 2006. Estimating long term urban exposure to particulate matter and ozone in Europe, Environmental Modelling and Software 21, 447-453.

Arvanitis A. and Moussiopoulos N. 2003. Coupling an aerosol module to a deterministic long term ozone exposure model. *26th NATO/CCMS ITM*, Istanbul

Kerschbaumer, A. and Reimer, E. 2003. Preparation of Meteorological input data for the RCG-model, UBA-Rep. 299 43246, Free Univ. Berlin Inst for Meteorology (in German)

Kunz R. and N. Moussiopoulos 1997. Implementation and assessment of one-way nesting technique for high resolution wind flow simulations. *Atmospheric Environment*, 31, 3167-3176.

Moussiopoulos N. and Douros I. 2004. Application and development of the OFIS model within the framework of CITYDELTA, *9th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes,* Garmisch-Partenkirchen, Germany, 1-4 June.

Sandnes Lenschow, H. and Tsyro, S. 2000. Meteorological input data for EMEP/MSC-W air pollution models, EMEP MSC-W Note 2/2000.

Schaap, M., Timmermans, R.M.A., Sauter, F.J., Roemer, M., Velders, G.J.M., Boersen, G.A.C., Beck, J.P. and Builtjes, P.J.H. 2005. The LOTOS-EUROS model: description, validation and latest developments, accepted in Int. J. of Environment and Pollution.

Simpson, D., Andersson-Sköld, Y. and Jenkin, M. E. 1993. Updating the chemical scheme for the EMEP MSC-W oxidant model : current status, Norwegian Meteorological Institute, EMEP MSC-W Note 2/93.

URL1: http://www.air4eu.nl

URL2: http://www.emep.int

EFFECTS OF DIFFERENT SURFACE PARAMETERIZATIONS ON MODEL PERFORMANCE IN URBAN AREAS

Sylvia I. Bohnenstengel[1], K. Heinke Schlünzen[2]
1) Max-Planck-Institut für Meteorologie, ZMAW, Hamburg, Bundesstr. 53, 20146 Hamburg, Germany, sylvia.bohnenstengel@zmaw.de
2) Meteorologisches Institut, ZMAW, Universität Hamburg, Bundesstr. 55, 20146 Hamburg, Germany heinke.schluenzen@zmaw.de, phone: +49-40-42838 5082 fax: +49-40-42838 5452

ABSTRACT

With increasing computing power resolutions of mesoscale atmospheric models increase. This does, however, not necessarily improve model performance as evaluations show. Especially, in very heterogeneous areas like urban areas, where sealed densely build areas and irrigated gardens and parks are present within the same grid box the aggregation effect impacts model performance. To ensure a good forecast of concentrations of pollutants an accurate prediction of the flow field and the vertical mixing is essential. Two schemes to parameterize sub-grid-scale surface fluxes are applied to the area around Berlin for different meteorological situations and grid resolutions. Parameter averaging and a flux aggregation method with blending height concept are validated for grid resolutions 4, 8 and 16 km. Model performance is determined by calculating hit rates from DWD routine data.

1. INTRODUCTION

The parameterization of surface fluxes with inclusion of sub-grid-scale land-use becomes very important in very heterogeneous areas like urban areas. Here are many different land-use types present within the same grid box. The so called “aggregation effect” (Giorgi and Avissar, 1997) affects the representativeness of the grid box averaged fluxes, since the system acts highly non-linear. In urban areas different land-use types, which are highly varying in their surface characteristics, are present within one grid box. A good forecast of concentrations does not only depend on emissions and chemical reactions, but also on the flow field. The latter is investigated for the area of Berlin. Like other urban areas the urban geometry result in lower wind speeds leading to a less intense vertical mixing in contrast to suburban or more rural areas. In the densely built areas the latent heat flux is lower than in suburban and rural areas resulting in high Bowen ratios. Thus, heat release is dependent on the intensity of the sensible heat flux and more heat is stored in the urban layer compared to rural areas leading to higher temperatures. However, within a grid box irrigated gardens or parks may result in a low Bowen ratio with an intense heat release due to the latent heat flux. Both extremes may occur in the same grid box. The contrary fluxes have to be represented by some kind of grid box averaged fluxes. Vertical exchange and flow field react sensitive to the parameterization applied for sub-grid-scale surface fluxes of heat and momentum. In addition, model performance depends on the resolution applied (Schlünzen and Katzfey, 2003).

2. METHODOLOGY

Two different parameterization schemes, flux aggregation with a blending height approach and parameter averaging, are applied to represent sub-grid-scale surface fluxes. They are evaluated for urban and rural areas. The resolution of 4, 8 and 16 km is applied for different meteorological situations and compared to DWD routine measurements of the basic variables like temperature, dew point, wind speed and wind direction. The four meteorological situations investigated differ in the influence of surface characteristics on the flow.

2.1 MODEL SET_UP

The 3D-simulations are undertaken for a very heterogeneous and flat area in Northern Germany (Figure 1), which has the advantage that orographically induced effects are of minor relevance. In the regions centre Berlin is situated with four urban measurement sites.

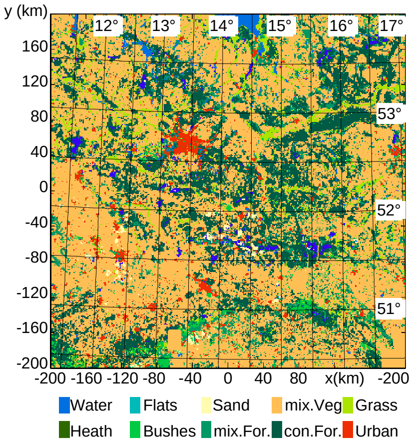

Figure 1. Land use in the model area.

Date	Grid sizes	I_{lt}	Additional characteristics
21.07.1974	18 km, 4 km	0	very dry situation
04.03.2003	16 km , 8 km , 4 km	10	humid situation
10.03.2003	16 km , 8 km , 4 km	30	very dry situation
03.06.2003	16 km , 8 km , 4 km	40	very dry situation

Table 1. Situations simulated.

Details on the model can be found in Schlünzen (1990), Dierer et al. (2005), Schröder et al. (2006). Here we focus on the parameterizations relevant for properly calculating surface fluxes. The vertical exchange coefficients are calculated with a mixing length approach for stable, neutral and slightly unstable stratification. A counter gradient scheme is used for convective situations (Lüpkes and Schlünzen, 1996) to correct turbulent heat flux in convective conditions, where large-eddy turbulent motion can produce a heat flux counter to the direction of the local temperature gradient (Holtslag and Moeng 1991). Two parameterization schemes are alternatively applied to calculate surface fluxes, a parameter averaging scheme and a flux aggregation method with blending height approach (von Salzen et al., 1996). Both can be applied to calculate area averages of the scaling values friction velocity u_*, free convection velocity w_* and the scaling value for the virtual potential temperature θ_{v*}. The heterogeneous sub-grid-scale land-use is incorporated using 10 fractional land-use classes per grid cell.

When using parameter averaging, surface properties like u_*, w_* and θ_{v*} are not calculated separately for each sub-grid-scale land-use class, but are derived using e.g. an effective roughness length z_0. This z_0 (eq. 1) is an artificial homogeneous roughness length representative for each grid box. The same averaging is applied for the other surface characteristics, like thermal diffusivity.

$$z_0 = \sum_{i=1}^{n} f_i z_{0i} \qquad (1)$$

This method has the advantage to be very cost-efficient and it performs quiet well as long as the surface characteristics are not too distinct (different kinds of bushes). Problems may arise when an area with a large fractional coverage connected with a marginal flux is next to a small area with a large flux. In theses cases, the grid box flux based on averaged parameters might be overestimated or even have the wrong direction.

This problem should be solved when applying the more expensive flux aggregation method using a blending height concept (von Salzen et al., 1996). Here the sub-grid-scale surface fluxes are calculated for each land-use class based on the class specific roughness lengths for momentum, temperature and humidity. As an example the latent heat flux is given in eq. (2).

$$\begin{aligned}\rho l_{21} q_* u_* &= \rho l_{21} \sum_{i=1}^{n} f_i\, q_{*i}\, u_{*i} \\ &= \rho l_{21} \kappa^2 U(z_1) \qquad (2) \\ &\cdot \sum_{i=1}^{n} f_i \cdot \left(q(z_1) - q(z_{0qi})\right) \cdot \left[\left(\ln\left(\frac{z_1}{z_{0i}}\right) - \psi_m\left(\frac{z_1}{L_i}\right)\right) \cdot \left(\ln\left(\frac{z_1}{z_{0qi}}\right) - \psi_q\left(\frac{z_1}{L_i}\right)\right)\right]^{-1}\end{aligned}$$

Specific humidity is denoted by q, U(z) is the main flow in x-direction at height z_1, ψ_m and ψ_q are the stability functions for momentum and humidity according to Dyer (1974). The von Kárman constant κ is set equal to 0.4. The sub-grid-scale surface fluxes are then averaged to a box averaged flux at the blending height l_{21}, which is the height, where the influence of the individual surface characteristics is blended out.

2.2 SIMULATED SITUATIONS

The 3D version of the atmospheric MEsoscale TRAnsport and Stream model METRAS (Schlünzen, 1990) is initialized with 1D background profiles assuming horizontal homogeneity. The simulations are nested in European wide observational data based on soundings and surface observations using a nudging approach. Table 1 summarizes the situations simulated. The selected situations differ by the influence of surface fluxes. This is characterized by the locality index I_{lt}. I_{lt} is a measure for the locality of the meteorological situation (Bohnenstengel and Schlünzen, 2007), describing how relevant local influences might be for the selected day.

2.3 RESULT EVALUATION

The model performance is evaluated by calculating hit rates from routine data of the four DWD stations in the Berlin area. The model results of temperature, dew point, wind speed and wind direction are interpolated to the location of the DWD stations at 2 m height above the surface. The hit rates are calculated following eq. (3):

$$H = \frac{100}{m}\sum_{i=1}^{m} n_i, \quad \text{with} \begin{cases} 1 \text{ for} \mid \text{difference}(\text{measurement}, \text{model}) \mid < A \\ 0 \text{ for} \mid \text{difference}(\text{measurement}, \text{model}) \mid \geq A \end{cases} \tag{3}$$

The desired accuracy A for temperature and dew point is set to +/- 2°K, for wind speed 1 ms^{-1}, for wind direction +/- 30° and for Pressure +/- 1.7 hPa.

3. RESULTS AND DISCUSSION

In general, flux aggregation with blending height performs better than parameter averaging in nearly all cases, for all resolutions and for all parameters. This is true for rural as well as for urban stations. For case $I_{lt}10$, which has a relatively large humidity, this conclusion is not fully supported. For wind direction and dew point temperature a clear decision for one or the other parameterisation is not supported by the model results.

Independent of the parameterization applied the simulation of wind speed is better for the rural areas than for the urban sites. The same is true for the dew point temperature and I_{lt} values of 10 and larger. For the $I_{lt}0$ case this is only true when using the flux aggregation with blending height method. Wind direction is somewhat better simulated for the urban sites ($I_{lt}10$, and $I_{lt}0$) and for larger I_{lt} values wind direction is better simulated for the rural sites. However, differences are small here.

Increasing the resolution mostly pays back for the urban sites. The performance improves for wind direction and wind speed. For temperature and dew point temperature an improvement with increasing resolution is also consistently found when using parameter averaging. For the flux aggregation method temperature (case $I_{lt}30$) or dew point temperature (case $I_{lt}0$) are not improved with increasing resolution. In addition, this parameterisation does not necessarily improve model performance when increasing the resolution from 8 to 4 km.

Increasing resolution for the rural sites results in very heterogeneous model answers. Parameter averaging tends to deliver better results when using higher resolution. Case $I_{lt}40$, however, shows a reduced model performance in wind direction and dew point temperature when increasing the resolution.

The humidity in the lower boundary layer plays a significant role in the model performance. For the relatively dry cases $I_{lt}40$, $I_{lt}30$ and $I_{lt}0$ model performance is better in rural areas for nearly all parameters than in urban areas. For the wet case $I_{lt}10$, model performance for the urban area is much better for wind direction and temperature than for the rural area.

4. CONCLUSIONS

Four case scenarios were simulated for different model configurations to determine the performance of two parameterization schemes for sub-grid-scale surface fluxes. In general, differences between the two schemes (flux aggregation with a blending height concept and parameter averaging) are found. Better performance of flux aggregation compared to parameter averaging is the general outcome. In addition, results are better for rural than for urban sites and can be improved for urban sites when using flux aggregation. Both methods seem to be resolution dependent, although flux aggregation is less resolution-dependent than parameter averaging. Still, we could not determine the best parameterization for each situation, since dynamic parameters and thermodynamic parameters perform different for the same case. Too many factors like the forcing via a nudging technique with an own analysis as well as the interpolation of the model results towards the routine observation stations influence the evaluation. To derive a conclusion that is independent of shortcomings of single simulations many more case studies are necessary.

5. ACKNOWLEDGEMENTS

This work is partly funded by the German Science Foundation under SCHL 499/1-1 and is a contribution to COST728.

6. REFERENCES

Bohnenstengel, S.I. and K.H. Schlünzen, 2007. A locality index to classify meteorological situations with respect to precipitation. (submitted to Journal of Applied Meteorology and Climatology)

Dierer S., Schlünzen K.H., Birnbaum G., Brümmer B., Müller G., 2005. Atmosphere-Sea Ice Interactions during Cyclone Passage Investigated by Using Model Simulations and Measurements. Month. Wea. Rev., 133, No.12, 3678-3692.

Dyer, A., 1974. A review of flux-profile relationship. Boundary Layer Meteorology, 7, pp. 362–372.

Giorgi, F. and R. Avissar, 1997. Representation of heterogeneity effects in earth system modeling: experience from land surface modeling. Reviews of Geophysics, 35(4), pp. 413–438.

Holtslag, A.A.M. and Moeng, C.H., 1991. Eddy diffusivity and countergradient transport in the convective atmospheric boundary layer, J. Atmos. Sci., 48, pp. 1690-1698.

Lüpkes, C., and K.H. Schlünzen, 1996. Modelling the Arctic convective boundary-layer with different turbulence parameterizations, Boundary-Layer Meteorol., **79**, 107-130.

Schlünzen K.H. and J.J. Katzfey, 2003. Relevance of sub-grid-scale land-use effects for mesoscale models. Tellus, 55A, pp. 232–246.

Schlünzen, K.H., 1990. Numerical studies on the inland penetration of sea breeze fronts at a coastline with tidally flooded mudflats, Beitr. Phys. Atmosph., 63, 243-256.

Schröder G., Schlünzen K.H., Schimmel F., 2006. Use of (weighted) essentially non-oscillating advection shemes in the mesoscale model. Quarterly Journal Roy. Met. Soc. 132, 1509-1526.

von Salzen K., Claussen M., Schlünzen K.H., 1996. Application of the concept of blending height to the calculation of surface fluxes in a mesoscale model. Meteorol. Zeitschrift, NF 5, 60-66.

INFLUENCE OF DIFFERENT PBL SCHEMES ON OZONE PREDICTIONS OVER THE GAA

[1]Elissavet Bossioli, [1]Maria Tombrou, [1]Aggeliki Dandou, [1]Eleni Athanasopoulou, [1]Kostas V. Varotsos
[1]National and Kapodistrian University of Athens, Department of Physics, Division of Applied Physics, Laboratory of Meteorology

Abstract
This study examines the influence of different PBL schemes on the ozone formation by coupling the meteorological MM5 model with the UAM-V model. The meteorological fields, which have been used in order to drive the photochemical simulations, derived from five different PBL schemes: the MRF, the Blackadar's, the Gayno-Seaman, the Pleim-Xiu schemes, plus a modified version of MRF scheme whereby urban features are considered. It was revealed that the sensitivity of the ozone patterns on the different PBL schemes is pronounced in the periphery of the basin during the afternoon hours. The formation of the peak ozone concentrations is not very sensitive to the different parameterizations of the PBL. However, although all PBL schemes predict similar daily maximum ozone concentrations, the size of their spatial extension differs. The MRF and MRF-urban schemes affect larger areas of the domain while Pleim-Xiu the smaller.

1. INTRODUCTION

Planetary boundary layer (PBL) and land-surface processes have critical implications on air quality simulations. The treatment of the evolution and structure of the boundary layer in meteorological models has important implications for predicting and understanding the dynamics of ozone and other photochemical pollutants (Ku et al., 2001; Mao et al., 2006) especially over complex topographies (Pérez et al., 2006). In the study of Bossioli et al., (2007) it was shown that the performance of the MM5/UAM-V modeling system over the Greater Athens Area (GAA) during an ozone episode strongly depends on the meteorological fields. The present study analyzes further the sensitivity of the MM5/UAM-V modeling system to different surface PBL parameterization schemes.

2. METHODOLOGY

The photochemical simulations were performed with the three-dimensional photochemical Urban Airshed Model, UAM-V (SAI, 1999) coupled with the PSU/NCAR Mesoscale Model (MM5) (Grell et al., 1994), version V3-6-1. Four different PBL approaches were considered: a) the high resolution non-local MRF scheme (Hong and Pan, 1996), based on the Troen and Mahrt's (1986) representation for counter-gradients and K-profiles in the well-mixed convective boundary layer; b) the high resolution Blackadar's (BL) scheme (Zhang and Anthes, 1982); c) the Gayno-Seaman (GS) scheme (Ballard et al., 1991), based on Mellor-Yamada TKE and d) the more recent Pleim-Xiu (PX) scheme (Pleim and Chang., 1992), a derivative of the Blackadar PBL scheme which uses a variation on the non-local vertical mixing. An additional simulation was also performed with a modified version of the MRF scheme, the MRF-urban PBL scheme (Dandou et al., 2005), where recent advances in the urban boundary layer are considered. In all the numerical simulations, additional updated fields for different parameters, such as the roughness length, albedo, thermal inertia, emissivity and moisture availability were also considered. This was achieved by applying an aggregation method in combination with detailed information derived from satellite image analysis (Landsat 5 Thematic Mapper image), with high spatial resolution (30m). The photochemical model was also modified in order to incorporate the updated fields of albedo and roughness length. Among the examined PBL schemes, BL and PX do not provide the diffusion coefficients for the unstable cases. In these cases the O'Brien (1970) method was applied directly to both sets of meteorological results.

The MM5 numerical simulations were performed by applying the two-way nesting. The coarse domain covers the extended area of Greece, with spatial resolution 6x6km, and the second domain is centred on the Attiki peninsula, with spatial resolution 2x2km. The photochemical model applied over the nested domain with spatial resolution 2x2km. The modelling system MM5/UAM-V was applied during an ozone episode where an open anticyclone prevailed.

3. RESULTS AND DISCUSSIONS

The simulations revealed that inside the city core the MRF scheme produces the highest ozone concentrations during most of the day. However, during the transition periods the MRF-urban scheme produces higher ozone concentrations in most urban and suburban stations, compared with the MRF scheme. This result is associated with the limitation of the ozone titration induced from higher diffusion coefficients calculated by the MRF-urban scheme (Tombrou et al., 2006).

In Figure 1a the spatial distribution of the mean hourly ozone concentrations predicted by the MRF scheme is presented at 1500LST while in Figures 1b-f the spatial distribution of the daily maximum 1-h ozone concentration at each grid cell over the modeling domain is presented for all PBL schemes. In all cases the location of the simulated peak concentrations is observed in the northern part of the basin. While all PBL schemes predict similar daily maximum ozone concentrations ranging between 75-85ppb, the size of their spatial extension differs. The MRF and MRF-urban schemes affect larger areas in total while PX the smaller. The MRF-

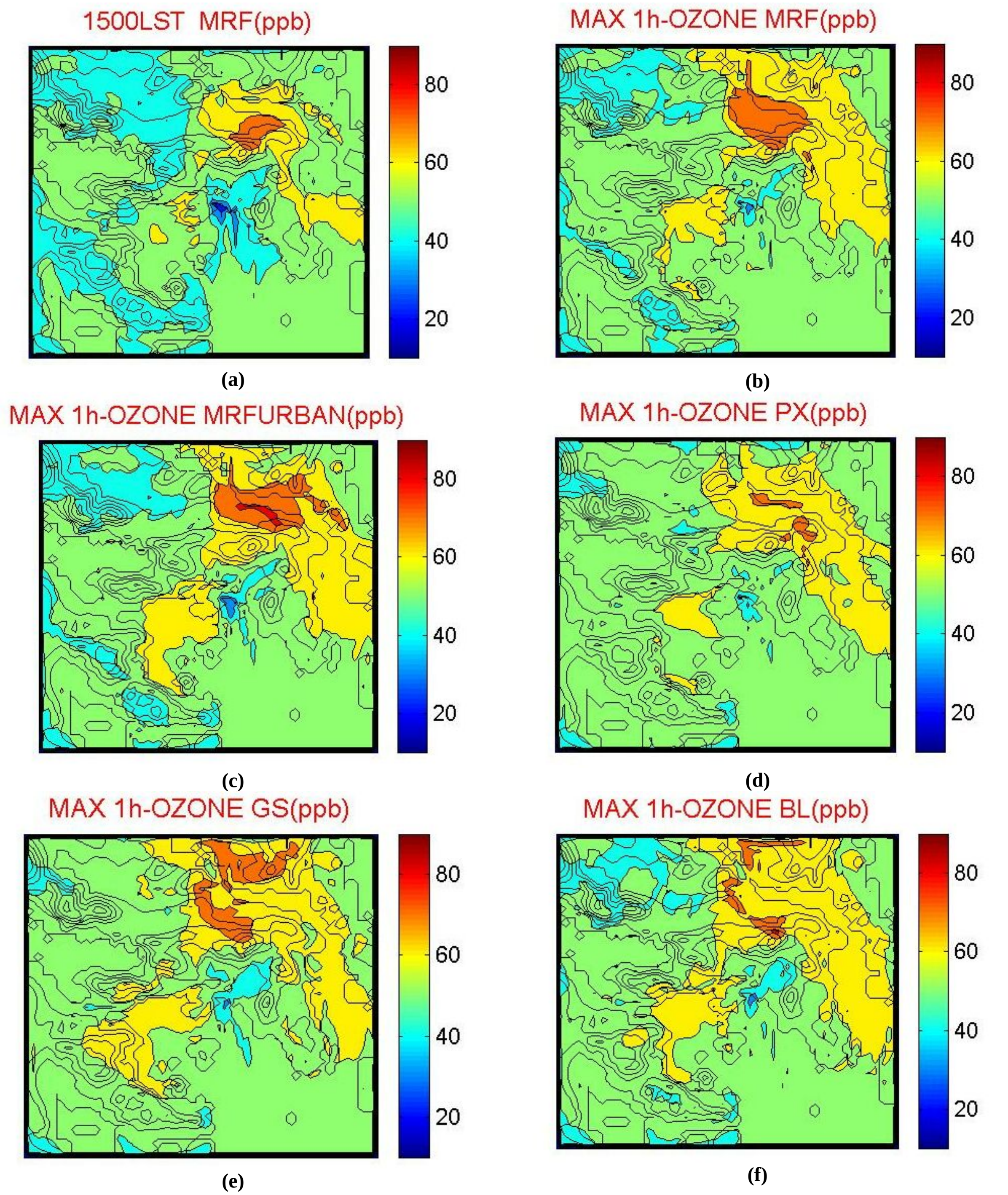

Figure 1: a) Spatial distribution of the mean 1-h ozone concentrations for the MRF scheme at 1500LST and (b)-(f) Spatial distribution of the maximum 1-h ozone concentration at each grid cell over the modeling domain for all PBL schemes.

urban and BL schemes predict higher daily maximum 1-h ozone concentrations in comparison to MRF, but not greater than 3%. The GS and PX schemes predict lower maximum values that reach 1% and 9% respectively.

The sensitivity of the ozone patterns on the different PBL schemes was found significant in the periphery of the basin during the afternoon hours. The spatial distribution of the differences of the mean hourly ozone concentrations between each scheme and MRF scheme at 1500LST is presented in Figure 2. It is evident that the BL and GS schemes produce higher concentrations compared to the MRF in the NW of the city center. The differences are equal to 15ppb and 10ppb for GS and BL schemes respectively and are due to the lower diffusion coefficients calculated by these schemes. Moreover, the pattern of the ozone differences is strongly associated with the wind fields and the developed convergence zones. The negative differences (10-20ppb) in the NE of the city center are due to the lower wind speeds predicted by the MRF scheme at this hour. Nevertheless, it is important to mention that most of the schemes produce higher ozone concentrations at these areas during later hours.

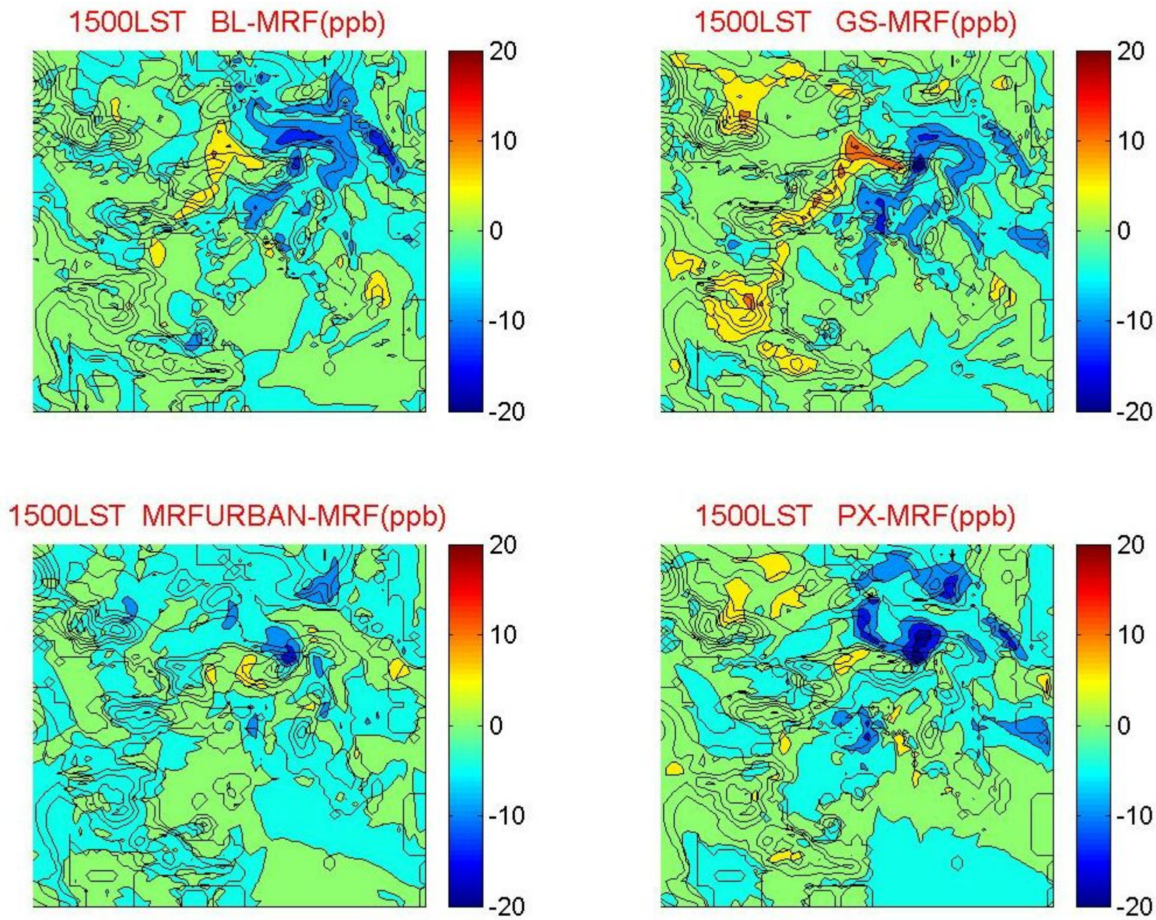

Figure 2: Spatial distribution of the differences of the mean 1-h ozone concentrations between each scheme and the MRF scheme at 1500LST.

4. CONCLUSIONS

The application of the MM5/UAM-V modeling system with different PBL schemes in the GAA revealed that the peak ozone concentrations are not very sensitive to the different parameterizations of the PBL. However, although all PBL schemes predict similar daily maximum ozone concentrations, the size of their spatial extension differs. In particular, the MRF and MRF-urban schemes affect larger areas of the domain while the PX the smaller.

The sensitivity of the ozone patterns on the different PBL schemes is pronounced in the periphery of the basin during the afternoon hours. The GS and BL schemes predict the highest concentrations and are due to the low values of the diffusion coefficients calculated by these schemes. For complete conclusions other synoptic conditions should also be studied.

5. ACKNOWLEDGEMENTS

We are grateful to the COST Action 728 'Meteorological parameterization/applications' activities which actually inspired this study.

6. REFERENCES

Ballard, S. P., Golding, W., and Smith, R. 1991, Mesoscale model experimental Forecasts of the Haar of the Notheast Scotland. Mon. Wea. Rev. 119, 2107-2123.

Bossioli, E., Tombrou, M., Dandou, A., Soulakellis, N. 2007. Simulation of the effects of critical factors on ozone formation and accumulation in the greater Athens area, J. Geophys. Res. 112, D02309.

Dandou, A., Tombrou, M., Akylas, E., Soulakellis, N., and Bossioli, E. 2005. Development and evaluation of an urban parameterization scheme in the Penn State/NCAR Mesoscale Model (MM5). J. Geophys. Res. 110, D10102, doi:10.1029/2004JD005192.

Grell, G. A., Dudhia, J., and Stauffer, D. 1994. A description of the fifth-generation pess state/NCAR mesoscale model (MM5). NCAR technical note, NCAR/TN-398+STR, 138 pp.

Hong, S.-Y., and Pan, H.-L. 1996. Nonlocal Boundary-Layer vertical diffusion in a medium-range forecast model. Mon. Wea. Rev. 124, 2322-2339.

Ku, J.-Y., Mao, H., Zhang, K., Civerolo, K., Rao, S. T., Philbrick, C. R., Doddridge, B., Clark, R. 2001. Numerical Investigation of the Effects of Boundary-Layer Evolution on the Predictions of Ozone and the Efficacy of Emission Control Options in the Northeastern United States. Environmental Fluid Mechanics 1, 209–233.

Mao, O., L.L. Gautney, T.M. Cook, M.E. Jacobs, S.N. Smith and J.J. Kelsoe (2006), Numerical experiments on MM5–CMAQ sensitivity to various PBL schemes Atmospheric Environment, 40, Issue 17, 3092-3110

O'Brien, J.J. 1970. A note on the vertical structure of the Eddy Exchange Coefficient in the Planetary Boundary Layer. J. Atmos. Sci. 27, 1213–1215.

Pérez, C., Jiménez, P., Jorba, O., Sicard, M., Baldasano, J.M., (2006), Influence of the PBL scheme on high resolution photochemical simulations in an urban coastal area over the Western Mediterranean. Atmospheric Environment, 40, 5274-5297

Pleim, J. E., and Chang, J. S. 1992. A non-local closure model for vertical mixing in the convective boundary layer. Atmos. Environ. 26A, 965-981.

SAI (1999), User's Guide to the Variable-Grid Urban Airshed Model (UAM-V), SYSAPP-99-95/27r3, Systems Applications International, San Rafael, CA.

Tombrou, M., Dandou, A., Helmis, C., Akylas, E., Angelopoulos, G., Flocas, H., Assimakopoulos, V., Soulakellis, N. 2006. Model evaluation of the atmospheric boundary layer and mixed-layer evolution. Boundary-Layer Meteorol. DOI 10.1007/s10546-006-9146-5.

Troen, I., and Mahrt, L. 1986. A simple model for the atmospheric boundary layer: Sensitivity to surface evaporation. Boundary- Layer Meteor. 37, 129-148.

Zhang, D., and Anthes, R.A. 1982. A high-resolution model of the planetary boundary layer- Sensitivity tests and comparisons with SESAME-79 data. J. Appl. Meteorol. 1594-1609.