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pollution in Lebanon**

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# Modeling air pollution in Lebanon: evaluation at a suburban site in Beirut

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## Abstract

Beirut, the capital city of Lebanon, which is located on the eastern shore of the Mediterranean basin, experiences high air pollution episodes. Annual average concentrations of coarse and fine particulate matter (PM<sub>2.5</sub>) as well as nitrogen oxides (NO<sub>x</sub>) often exceed the World Health Organization (WHO) guidelines. Therefore, improving air quality in this region is essential. The Polyphemus/Polair3D modeling system is used here to investigate air pollution episodes in Beirut during 2–18 July 2011. The modeling domain covers two nested grids of 1 and 5 km horizontal resolution over the greater Beirut and Lebanon, respectively. The anthropogenic emission inventory was developed earlier (Waked et al., 2012). The Weather and Research Forecasting (WRF) model is used to generate the meteorological fields and the Model of Emissions of Gases and Aerosols from Nature (MEGAN) is used for biogenic emissions. The results of the study are compared to measurements from a field campaign conducted in the suburb of Beirut during 2–18 July 2011. The model reproduces satisfactorily the concentrations of most gaseous pollutants, the total mass of PM<sub>2.5</sub> as well as PM<sub>2.5</sub> elemental carbon (EC), organic carbon (OC), and sulfate.

## 1 Introduction

The Middle East region is characterized by a diverse landscape including elevated terrain, semi-arid and Saharan deserts, sea shores and vast plains. Covering fourteen Arab countries as well as Turkey and Iran, the region stretches from Egypt in the West to Iran in the East, Turkey in the North and the Arabian Peninsula in the South. Being an enclosed region, it experiences high pollution episodes, elevated particulate matter (PM) concentrations and major acid deposition problems (Saliba et al., 2006 and references therein). Moreover, anthropogenic emissions are increasing rapidly over this region due to large industrialized areas, the absence of any efficient public transport system, dense traffic areas and high population densities (ESCWA, 2010; Lelieveld

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et al., 2009). In addition, steady winds originating from eastern Europe as well as intense solar radiation contribute to the formation of high levels of secondary pollutants and other reactive species (Lelieveld et al., 2002; Kouvarakis et al., 2000). To date, few studies have been conducted to investigate air pollution in this region. Lelieveld et al. (2002, 2009) and Smoydzin et al. (2012) investigated ozone (O<sub>3</sub>) pollution over the Middle East region and the Arabian Peninsula. The results showed that in the Arabian Peninsula, high levels of O<sub>3</sub> concentrations were observed especially in summer (Liu et al., 2009) due to the highly favorable weather conditions and high local air pollutant emissions (Lelieveld et al., 2009). In particular, nitrogen oxides (NO<sub>x</sub>) concentrations in this area are exceptionally high (Stavrakou et al., 2008). As a result, air pollution in this region needs to be investigated, monitored, and reduced. Lebanon, a small developing country in the Middle East region, located on the eastern shore of the Mediterranean Sea, experiences high pollution episodes due to local emissions because of a growing population, especially in urban areas, the absence of any public transport system (MoE, 2005), steady winds from eastern Europe and Saharan dust storms from the desert (Saliba et al., 2007). Therefore, the country represents a good case study for investigating air pollution in the region. The few measurements conducted in Beirut, the capital city of Lebanon, revealed high levels of nitrogen dioxide (NO<sub>2</sub>) with an annual average concentration of 66 μg m<sup>-3</sup> (Afif et al., 2009) and high levels of particulate matter, PM<sub>10</sub> and PM<sub>2.5</sub>, with annual concentrations of 64 and 20 μg m<sup>-3</sup>, respectively (Massoud et al., 2011). The levels exceed World Health Organization (WHO) guideline values of 40 μg m<sup>-3</sup> for NO<sub>2</sub> and 20 and 10 μg m<sup>-3</sup> for PM<sub>10</sub> and PM<sub>2.5</sub>, respectively. Although these measurements provide valuable information on air pollution, they are scarce and limited to a few areas. Therefore, the use of chemical-transport models (CTM) is essential for understanding the spatio-temporal distribution of gaseous and particulate pollutants in the region. Previous studies have focused on simulating the distribution of O<sub>3</sub> over this region using regional CTM. The EMAC chemistry general circulation model (Roeckner et al., 2006) was used to investigate O<sub>3</sub> levels in the Persian gulf region (Lelieveld et al., 2009) and a fully coupled on-line model (WRF-Chem

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version 3.3.1) (Grell et al., 2005) was used for the Arabian Peninsula (Smoydzin et al., 2012). However, no modeling study has yet been conducted for Lebanon or its capital city Beirut. In this study, the WRF-ARW version 3.3 meteorological model (Skamarock et al., 2008) is used with the Polyphemus/Polair3D CTM (Mallet et al., 2007; Sartelet et al., 2007) to investigate air pollution in Beirut as well as in Lebanon from 2 till 18 July 2011. WRF has been evaluated against observations in many regions (Borge et al., 2008; Carvalho et al., 2012; Molders, 2008) but, to our knowledge, has never been applied to Lebanon. The Polyphemus/Polair3D CTM has been evaluated over Europe (Sartelet et al., 2007, 2012; Couvidat et al., 2012), Asia (Sartelet et al., 2008), and North America (Sartelet et al., 2012), but not in the Middle East region. This study aims to investigate air pollution in Beirut in July 2011 via meteorological and air quality modeling. The evaluation of WRF and Polyphemus/Polair3D in this region is essential prior to the use of such models for future air quality studies.

The methodology and the model configurations for WRF and Polyphemus/Polair3D are described in Sect. 2. The evaluation results for the meteorological and chemical simulations against observations are presented and discussed in Sects. 3 and 4, respectively. Conclusions are provided in Sect. 5.

## 2 Method

### 2.1 Modeling domains

For meteorological modeling, three modeling domains were set on a latitude-longitude projection. A mother domain (D3) with 25 km horizontal resolution covering the Middle East region, as well as some parts of eastern Europe, northern Africa and the Mediterranean Sea, and two nested domains with 5 km resolution for Lebanon (D2) and 1 km resolution for Beirut and its suburbs (D1) were adopted. The two nested domains D1 and D2 are used for the air quality model simulations.

## 2.2 Episode selection and observational data set

The modeling study was conducted from 2 till 18 July 2011. During this period, meteorological and air quality measurements were conducted at the Faculty of Sciences of the Saint Joseph University campus (USJ site) in the region of Mansourieh (33.86° N; 35.56° E) distant by 6 km from the center of Beirut. Meteorological measurements included wind speed (anemometer), wind direction (weather vane), surface temperature (thermometer), relative humidity (hygrometer) and atmospheric pressure (barometer). Average temperatures in Beirut exceeded 28 °C and clear skies were dominant. No precipitation was recorded during this period. These weather conditions, as well as westerly and easterly winds coming from eastern Europe and Asia, respectively, favored oxidant and secondary organic aerosol (SOA) formation. Trace gases including carbon monoxide (CO), NO<sub>x</sub> and O<sub>3</sub> were measured on-line on a 1-min basis using trace gas analyzers (Michoud et al., 2012) while VOC were measured on a 1-h basis using an on-line Thermal Desorption Gas Chromatography with a Flame Ionization Detector (TD-GC-FID) and on a 5-min basis using a Proton Transfer Reaction Mass Spectrometry (PTRMS). However only, the results obtained from the TD-GC-FID are used for the evaluation of modeled VOC. PM<sub>2.5</sub> samples were collected using a high-volume sampler (30 m<sup>3</sup> h<sup>-1</sup>) on a 12-h basis. They were analyzed for OC and EC using the EU-SAAR2 protocol (Cavalli et al., 2010), for organic aerosols using a gas chromatography coupled to a mass spectrometry (GC/MS) technique and for inorganic aerosols using an ion chromatography (IC) technique. The model simulation results are compared with those measurements to evaluate the ability of the model to reproduce major chemical components of photochemical air pollution in Beirut.

## 2.3 Meteorological modeling

WRF-ARW was used to generate the meteorological fields using a two-way nesting approach with a vertical structure of 24 layers covering the whole troposphere. Initial and boundary conditions were driven by the National Centers for Environmental Prediction

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(NCEP) global tropospheric analyses with  $1^{\circ} \times 1^{\circ}$  spatial resolution and 6 h temporal resolution. Topography and land use were interpolated from the United States Geological Survey (USGS) global land covers with the appropriate spatial resolution for each domain.

Physical parameterizations used in the model include the Kessler microphysics scheme (Kessler, 1969), the RRTM long-wave radiation scheme (Mlawer et al., 1997), the Goddard NASA shortwave scheme (Chou and Suarez, 1994), the Grell-Devenyi ensemble cumulus parameterization scheme (Grell and Devenyi, 2002) and the Noah land surface model (Chen et al., 2001). Several physical options such as planetary boundary layer (PBL) dynamics, land surface model as well as several numerical options are available in WRF. A series of model experiments changing one option at a time was conducted to identify the simulation which provides the lowest biases and errors when compared to the observations. Because meteorological models tend to diverge after some integration time (typically two or three days), segmented simulations were also performed. Thus, several two-day restarted simulations were performed to complete an 18 day long simulation. For each simulation, the first 12-h period was considered as a spin-up period for the model. Because the PBL has an important impact on the near surface wind field, two PBL schemes were tested: the Yunsai University (YSU) PBL scheme (Hong et al., 2006), which is a non-local closure scheme (Stull, 1988) and the Mellor-Yamada-Nakanishi and Niino (MYNN) level 2.5 scheme (Nakanishi and Niino, 2004), which is a local TKE-based scheme. The MYNN scheme was developed to improve performance of its original Mellor-Yamada model (Mellor and Yamada, 1974). Major differences between the two schemes (MYNN and MY) are the formulations of the mixing length scale and the method to determine unknown parameters. In addition, because the inner domain (D1) includes large urban areas, an urban surface model was used. WRF includes three urban surface models: the urban canopy model (UCM) (Kusaka et al., 2001), which is a single layer model, and two multi-layer models, the Building Environmental Parameterization (BEP) (Martilli et al., 2002) and the Building Energy Model (BEM) (Salamanca et al., 2010). In this study, UCM was used because it

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includes the anthropogenic heat release, which is not included in the multi-layer models (Kim, 2011). Using UCM, several influential parameters such as the anthropogenic heat flux, road width, and building width and height values typical for Beirut were chosen, whereas for other parameters (urban ratio for a grid, surface albedo of roof, road and wall, thermal conductivity of roof, road and wall, etc.), the values provided by the WRF configuration file were adopted because of a lack of data. Therefore, a reference building width of 11 m (CBDE, 2004) and a road width of 8.5 m were adopted (Chélala, 2008). A building height of 17.9 m was chosen (Chélala, 2008) while the mean annual anthropogenic heat flux (the heat released to the atmosphere as a result of human activities) for Beirut was estimated to be  $17 \text{ W m}^{-2}$  (IIASA, 2012).

## 2.4 Air quality modeling

The Polyphemus/Polair3D CTM was used. Aerosol modeling was performed using SIREAM (Size Resolved Aerosol Model) (Debry et al., 2007) coupled to the Hydrophilic/Hydrophobic Organic ( $\text{H}^2\text{O}$ ) model for SOA formation (Couvidat et al., 2012), ISORROPIA (Nenes et al., 1998) for inorganic aerosols thermodynamics, and the CB05 chemical kinetic mechanism for gas-phase chemistry (Yarwood et al., 2005; Kim et al., 2009, 2011). SIREAM segregates the particle size distribution into sections and solves the general dynamic equation by splitting coagulation and condensation/evaporation-nucleation (Debry et al., 2007). In  $\text{H}^2\text{O}$ , two anthropogenic and five biogenic SOA precursors species are used as surrogate precursors. In order to account for the fact that primary organic aerosols (POA) are semi-volatile organic compounds (SVOC), an SVOC/EI-POA (Emissions Inventory based POA) value of 5 was adopted following Couvidat et al. (2012) to estimate SVOC emissions.

The USGS land cover was used. Initial and boundary conditions for the outer domain (D2) were extracted from the output of the Model for Ozone And Related chemical Tracers version 4 (MOZART-4; <http://www.acd.ucar.edu/wrf-chem/mozart.shtml>), which is an off-line global tropospheric CTM (Emmons et al., 2010). It is driven by NCEP/NCAR reanalysis meteorology and uses emissions based on a database of surface emissions

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of ozone precursors (POET), Regional Emission Inventory in Asia (REAS) and Global Fire Emissions Database (GEFD2). The results are at  $2.8^\circ \times 2.8^\circ$  horizontal resolution for 28 vertical levels. It should be noted that a pre-simulation was performed for the D1 (24 June till 2 July) and D2 (15 June till 2 July) domains to eliminate the effect of initial conditions. Outputs from the meteorological model (WRF-ARW) were used to compute vertical diffusion with the Troen and Mahrt (1986) and Louis (1979) parameterizations within the PBL. For horizontal diffusion, the CMAQ parameterization was used (Byun and Schere, 2004). Gas and particle deposition as well as sea-salt emissions were pre-processed using relevant meteorological variables. Biogenic emissions were calculated using the Model of Emissions of Gases and Aerosols from Nature (MEGAN V.2; Guenther et al., 2006). This model, which is designed for global and regional emission modeling, has a global coverage with a  $1 \text{ km} \times 1 \text{ km}$  resolution.

For anthropogenic emissions, a spatially-resolved and temporally-allocated emission inventory was developed for Lebanon as well as for Beirut and its suburbs in a previous study (Waked et al., 2012). This emission inventory is used here. Emissions were spatially allocated using a resolution of 5 km over Lebanon and a resolution of 1 km over Beirut. The inventory includes the emissions of CO, NO<sub>x</sub>, sulfur dioxide (SO<sub>2</sub>), VOC, ammonia (NH<sub>3</sub>), PM<sub>10</sub>, and PM<sub>2.5</sub>. A wide variety of emission sources including road transport, maritime shipping, aviation, energy production, residential and commercial activities, industrial processes, agriculture, and solvent use are included in this inventory. A bottom-up methodology was used for the major contributing sources such as road transport, cement industries and power plant energy production. For other sources, a top-down approach was adopted. Spatial allocation was performed using population density maps, land cover and road network as well as traffic count data and surveys in many regions (Waked and Afif, 2012). Temporal profiles were allocated with monthly, daily, and diurnal resolutions for all sources. The inventory was developed for a base year of 2010.

### 3 Meteorological simulations

#### 3.1 Model simulation configurations

The results obtained from WRF were evaluated with meteorological data collected at the USJ site. Reliable meteorological data at other locations were not available within the D1 and D2 domains, thereby preventing a more complete model performance evaluation. Different simulations from M1 to M5 (Table 1) were performed in order to select the meteorological simulation which has the lowest biases and errors when compared to observations.

For physical parameterizations, the YSU PBL scheme (simulation M2) and the MYNN scheme (simulation M3) were tested with the use of UCM. In addition, two simulations (M1 and M4) with the YSU and MYNN schemes, respectively, were performed without the use of UCM. To test numerical options, a simulation (M5) was performed using segmented simulations with two-day restarts to assess whether the model tends to diverge significantly after 2 days of simulation.

#### 3.2 Results

To evaluate a model, several approaches can be used (Gilliam et al., 2006). Here, we compare model simulation results to measurements at one site using model performance statistical indicators that include the root mean square error (RMSE), mean fractional bias (MFB), mean fractional error (MFE), normalized mean bias (NMB), normalized mean error (NME), and the correlation coefficient (see Supplement). The results of the statistical evaluation for wind speed and wind direction at 10 m above ground level (a.g.l.), surface temperature, relative humidity, and pressure at 2 m a.g.l. are presented in Table 2 for the five simulations tested. Overall, the model is able to reproduce local wind speed, surface air temperature, and pressure with correlations greater than 0.74 (simulation M1). For wind direction and relative humidity, lower correlations (0.2–0.4) are obtained. Wind speed and wind direction have values of MFB and NMB in

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the range of 20 to 60 %. For surface temperature, relative humidity, and pressure, the statistical biases indicate a low over-prediction of 1 to 10 %. Accordingly, RMSE reported values for surface temperature (1.54 °C) and wind speed (1.34 m s<sup>-1</sup>) are low, those of relative humidity (13 %) and pressure (14 hPa) are moderate, and that of wind direction is high (92°, simulation M1). Thus, model predictions of wind direction are the worst among the five variables. Other studies have shown RMSE values for surface temperature of 2.8 °C in Alaska (Molders, 2008), 3.46 °C in the southern US (Zhang et al., 2006), and 2.82 °C in Paris (Kim, 2011). For wind speed, these values were 3 m s<sup>-1</sup> in Portugal (Carvalho et al., 2012), 1.62 m s<sup>-1</sup> in the southern US (Zhang et al., 2006), and 1.93 m s<sup>-1</sup> in Paris (Kim, 2011). For wind direction, RMSE values of 92° are comparable to the value obtained in the southern US (97°, Zhang et al., 2006), but greater than the value obtained in Portugal (52°, Carvalho et al., 2012). Therefore, this meteorological simulation shows satisfactory performance when compared to other similar studies.

### 3.3 Numerical options

The evaluation of segmented simulations is reported in this section because grid nudging of the NCEP initial and boundary conditions was used in all simulations. Comparison between simulation M5 (segmented simulations with two-day restarts) and the other simulations (M1–M4) showed better correlations for all the variables for the long simulations without segmentation, especially for wind components where M5 gives correlations of 0.55 and 0.23 for wind speed and wind direction respectively, compared to values of 0.74 and 0.38 obtained from a long simulation without segmentation such as M1. For other variables, differences between simulations are not significant. RMSE and other statistical indicator values are comparable between M5 and the continuous simulations. This leads to the conclusion that the model does not diverge significantly after some integration time, which results in part from the small size of the D1 domain and its two-way nesting to greater domains. On the other hand, there is considerable uncertainty in the initial conditions, which are generated every two days in the

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non-continuous simulations because these initial conditions are provided with a spatial resolution of 100 km to be used in a simulation for Beirut with a spatial resolution of 1 km, thereby leading to biases and errors that are higher than those of a continuous simulation.

### 5 3.4 Physical parameterizations

The MYNN PBL scheme used with UCM (simulation M3) was found to produce the best statistical results for all the variables. Accordingly, this physical option influences wind speed, surface temperature, relative humidity, and pressure. Using this option leads to the best correlations among all the simulations for all variables except for wind speed. The correlations are 0.63, 0.39, 0.91, 0.31, and 0.97 for wind speed, wind direction, surface temperature, relative humidity, and pressure. For MFB, MFE, NMB and NME, no significant differences are observed among these simulations (M1–M4). In summary, M1 with the YSU scheme gives the best results for wind speed and M3 with the MYNN scheme and UCM gives the best results for wind direction and relative humidity.

### 3.5 Best configuration

Temporal variations for wind speed, wind direction, surface temperature, and relative humidity of the two best selected simulations (M1 and M3) are shown from 2 July, 00:00 till 17 July, 00:00, 2011 in Fig. 2 because after 17 July, 00:00, no observations were recorded. The model reproduces wind direction better from 6 till 10 July in both simulations while from 2 till 6 July and from 12 till 16 July, the model is not able to reproduce winds originating from the East. The model reproduces satisfactorily relative humidity for the selected period in simulations except on 4, 5, 15 and 16 July when the model over-predicts relative humidity. Surface temperature is better reproduced in simulation M3 than in simulation M1 which over-predicts surface temperature. Lastly, a comparable pattern is observed with lower values for wind speed in simulation M3 due

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to the use of UCM, which has an effect of decreasing wind speeds due to urbanization. In summary, the model performs better from 6 till 10 July for all the variables.

Clearly, the PBL scheme influences wind speed, wind direction, and surface temperature (Borge et al., 2008). Temperature is best modeled with the MYNN scheme using UCM. This result agrees with that obtained by Kim (2011) in a simulation over Paris, France. Outside the center of the city, the effect of UCM on temperature is not significant and is compensated by the effect of the PBL scheme. For wind speed and wind direction, no significant variation is observed between M1 and M3. For relative humidity, a better correlation is obtained using the MYNN PBL scheme, and a lower non-significant correlation is obtained for wind speed. Overall, simulation M3 performs slightly better for most variables than simulation M1 particularly for temperature and humidity and we may consider that the correlation of 0.63 obtained for wind speed in simulation M3 is close to the correlation of 0.74 (systematic error of 18 %) obtained in simulation M1 while the correlation for relative humidity of 0.31 obtained in simulation M3 is significantly different from the value of 0.2 (systematic error of 43 %) obtained in simulation M1. In addition, surface air temperature and wind direction were slightly better modeled in simulation M3 in terms of temporal variation (Fig. 2) and NMB (Table 2). Based on these considerations, the results obtained from simulation M3 are used for air quality modeling.

#### 4 Air quality simulations

The results obtained from Polyphemus/Polair3D were evaluated against measurements of gaseous species ( $O_3$ ,  $NO_2$ , VOC and CO) and  $PM_{2.5}$  (total mass and major components) collected at the USJ site. Statistical indicators used for model evaluation include MFB, MFE, mean normalized bias (MNB), and mean normalized error (MNE) (see Supplement).

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## 4.1 Gaseous species

The base simulation conducted with the MOZART-4 boundary conditions (A1) led to O<sub>3</sub> concentrations within the D1 domain that were too high compared to the observations by nearly a factor of two (see Table 3). Sensitivity simulations were conducted where emissions of NO<sub>x</sub> (A2) and VOC (A3) were reduced by a factor of two; these simulations did not lead to satisfactory O<sub>3</sub> concentrations, in part because of the strong influence of the boundary conditions. A decrease of NO<sub>x</sub> emissions leads to an increase in O<sub>3</sub> concentrations (A2) because the study area is saturated in NO<sub>x</sub>. Moreover, NO<sub>x</sub> concentrations are well reproduced by the model in the base simulation A1. VOC reductions are effective in reducing O<sub>3</sub> concentrations (A3) due to the fact that the area of the study is considered to be VOC-limited, having a VOC to NO<sub>x</sub> ratio in the range of 3 to 5. However, the decrease in O<sub>3</sub> concentrations is insufficient to match the observed concentrations and VOC concentrations are already underestimated by the model in A1 by a factor of 2 to 3 (Table 4). An increase of NO<sub>x</sub> emissions and a decrease of VOC emissions could lead to satisfactory O<sub>3</sub> concentrations, but would lead to non-satisfactory results for VOC and NO<sub>x</sub> modeled concentrations. Therefore, a sensitivity simulation was also conducted with the boundary O<sub>3</sub> concentrations halved (A4). That simulation led to reasonable agreement with the observations for all gaseous species. A comparison between simulation A1 and simulation A4 shows that modifying the O<sub>3</sub> boundary concentrations has negligible effect on CO, NO<sub>x</sub> and PM<sub>2.5</sub> modeled concentrations. Although a recent evaluation of MOZART-4 with ozone study led to satisfactory results (Emmons et al., 2010), a detailed evaluation with PBL O<sub>3</sub> data in the Middle East region has not been conducted because of a lack of data. Better characterization of PBL air pollution concentrations in that region is needed to obtain realistic O<sub>3</sub> boundary concentrations.

This strong influence of boundary conditions which leads to a significant overestimation of O<sub>3</sub> concentrations may be due to the fact that the MOZART-4 data used during this study have a horizontal resolution of 280 km and are used as boundary conditions

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for a domain D2 with a horizontal resolution of 5 km. It is possible that the use of an intermediate domain of 25 or 50 km horizontal resolution may decrease the uncertainties generated by the MOZART-4 data. However, an emission inventory for the Middle East region is not currently available and the use of an intermediate domain D3 for air quality simulation is therefore not feasible. In addition, we compared the results of this simulation to O<sub>3</sub> concentrations measured in the summer of 2004 in Beirut at an urban site (Saliba et al., 2006) in order to assess the accuracy of the simulation at a different location than the one where the measurements are performed. Such comparisons are not true evaluations of the model because the years of the simulation and observations differ. Nevertheless, such comparisons may point to some possible biases in the air quality simulation if the differences cannot be justified. The results show a modeled value of 1585 μg m<sup>-3</sup> for CO in both simulations A1 and A4 compared to a measured value of 1213 μg m<sup>-3</sup>. For PM<sub>10</sub>, a value of 47 μg m<sup>-3</sup> was modeled in both simulations compared to a measured value of 44 μg m<sup>-3</sup>. The modeled O<sub>3</sub> concentrations are 54 μg m<sup>-3</sup> in simulation A1 and 32 μg m<sup>-3</sup> in simulation A4, compared to a measured value of 34 μg m<sup>-3</sup>. Clearly, the results obtained from this evaluation show that simulation A4 with modified O<sub>3</sub> boundary conditions leads to better results for O<sub>3</sub> concentrations and has negligible effect on other pollutants. Therefore, simulation A4 is used below.

Average modeled surface concentrations (over both land and sea) of O<sub>3</sub>, NO<sub>2</sub>, and CO from 2 to 18 July are 50, 49 and 700 μg m<sup>-3</sup> in the inner domain (D1) and 72, 10 and 240 μg m<sup>-3</sup> in the outer domain (D2), respectively. The modeled surface spatial distributions of O<sub>3</sub> and NO<sub>2</sub> concentrations for D2 and D1 (Figs. 3 and 4) show lower O<sub>3</sub> concentrations where most NO<sub>x</sub> emissions from industries, harbors and road traffic occur and higher values in the mountains. Accordingly, higher concentrations of NO<sub>2</sub> are modeled near the coast in Beirut and its suburbs, in the cities of Tripoli and Chekka in the north and Jieh in the south. Major sources in those areas include dense traffic in urban areas and on highways along the coast, in particular in Beirut and Tripoli, the Zouk power plant located on the coast north of Beirut, the Jieh power plant and the

cement plants located in the city of Chekka. Other emissions are generated from the harbors in Beirut and Tripoli and from the international airport located on the coast south of Beirut. Higher O<sub>3</sub> concentrations modeled in the mountains (east of the domain) might be related to a higher VOC/NO<sub>x</sub> ratio (Fig. 5), which is more favorable to O<sub>3</sub> formation.

To evaluate the model concentration results at the USJ site, different statistical metrics were calculated for the 2–18 July period, as shown in Table 4.

The model reproduces satisfactorily O<sub>3</sub> concentrations (bias in the range of 9 to 17%). MNB and MNE values for O<sub>3</sub> of –9% and 33%, respectively, are within suggested performance criteria (Russel and Denis, 2000) of ±5–15% for MNB and 30–35% for MNE. The mean NO<sub>2</sub> concentration is well reproduced by the model but the hourly concentrations show a positive bias. For NO<sub>2</sub>, the MNB of 42% is comparable to the reported value of 35% obtained during a simulation in the North Sea coastal region in Europe in July 2001 (Matthias et al., 2008) and to the day-time and night-time values of –19% and 31% reported in Mexico City during the MCMA-2006/MILAGRO field campaign (Zhang et al., 2009). In addition, a MNB of 74% for NO<sub>x</sub> calculated during this study is in better agreement with observations than the reported value of 101% for a simulation over Nashville, USA, in July 1999 using the CMAQ model (Bailey et al., 2007). CO concentrations show an over-prediction by the model on the order of 30% on average. These results are comparable to those of other studies conducted in Europe, Mexico and the USA (Matthias et al., 2008; Zhang et al., 2009; Bailey et al., 2007). Biogenic VOC concentrations are small (< 1 µg m<sup>-3</sup>) for both observations and simulations; they show an over-prediction of α-pinene by the model by a factor of two and an under-prediction of isoprene on the order of 30% on average. However, the α-pinene model species is a surrogate species that includes α-pinene and sabinene. The MNB value of –14% reported for isoprene is comparable to the reported values of 14% and –17% during a simulation in July 2004 using the MOZART-4 CTM (Horowitz et al., 2007). Anthropogenic VOC such as toluene and xylene are under-estimated by the model by a factor of 2 to 3. Nevertheless, the results obtained are satisfactory because

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5 speciated VOC emissions are associated with large uncertainties and modeled VOC concentrations, which are typically not evaluated, are subject to significant bias. Indeed, monoterpene concentrations are underestimated by almost a factor of two in a simulation over the eastern US using the MOZART-4 CTM (Horowitz et al., 2007) due to a significant underestimation in terpene emissions while isoprene emission estimates can differ by more than a factor of 3 for specific times and locations when different driving variables are used in the emissions calculations (Guenther et al., 2006). Temporal variations for O<sub>3</sub> are shown in Fig. 6 from 2 till 13 July 2011 (no measurements were recorded after 13 July). The model reproduces satisfactorily the diurnal variation of O<sub>3</sub>, with a peak O<sub>3</sub> concentration occurring between 12:00 p.m. and 01:00 p.m. for both observed and modeled values on most days. However, on some days (2, 3, and 9 July), a second O<sub>3</sub> peak is observed between 09:00 a.m. and 10:00 a.m. This second peak is not reproduced by the model.

## 4.2 Particulate pollutants

15 Modeled PM<sub>2.5</sub> average surface concentrations (over both land and sea) from 2 to 18 July 2011 are 10 µg m<sup>-3</sup> for Lebanon (D2) and 19 µg m<sup>-3</sup> for Beirut and its suburbs (D1). The spatial distribution of PM<sub>2.5</sub> concentrations (Fig. 7) shows higher concentrations (> 40 µg m<sup>-3</sup>) in the city of Beirut and its northern suburb, Chekka in the north and Siblinge in the south. Dense on-road traffic, industrial sources (Zouk plant north of Beirut and the cement plants near the coast of Chekka and Siblinge) and Beirut international airport located south of Beirut lead to significant air pollutant emissions (Waked et al., 2012). Lower PM<sub>2.5</sub> concentrations in the eastern part of the domains (< 20 µg m<sup>-3</sup>), are related to the fact that anthropogenic sources in these areas are less significant. This suggests that PM<sub>2.5</sub> concentrations are dominated by anthropogenic sources. Indeed, biogenic modeled SOA account for only 4 % of total PM<sub>2.5</sub> modeled concentrations in the inner domain D1 and 8 % in the outer domain D2. Compared to the WHO annual guideline of 10 µg m<sup>-3</sup> and 24-h average guideline of 25 µg m<sup>-3</sup>, PM<sub>2.5</sub>

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concentrations exceed these values in large urban agglomerations such as Beirut and Tripoli and in the regions of Chekka and Sibline where several cement plants are located and modeled  $PM_{2.5}$  are above  $100 \mu g m^{-3}$ .

Statistical model performance at the USJ site is presented in Table 5. The observed value for  $PM_{2.5}$  is a reconstructed mass concentration based on the IMPROVE method (IMPROVE, 2011). Overall, the model reproduces satisfactorily  $PM_{2.5}$ , OC, EC, and sulfate ( $SO_4^{2-}$ ) average concentrations. MFB values in the range of  $-21$  to  $25\%$  and MFE values in the range of  $39$  to  $61\%$  obtained during this study indicate that the model meets the performance criteria ( $-60\% \leq MFB \leq +60\%$  and  $MFE \leq 75\%$ ) suggested by Boylan and Russel (2006). For nitrate and ammonium, there is a large underestimation of the model. This high underestimation could be related in part to uncertainties in  $NH_3$  emissions. On the other hand, the measured nitrate concentrations could be overestimated due to adsorption of nitric acid on the particulate filters because no denuder was placed upstream of the filters. The MFB and MFE reported values of  $-59\%$  and  $61\%$  obtained for OC during this study are in agreement with the values of  $-37\%$  and  $50\%$  reported for Europe in another simulation conducted using Polyphemus/Polair3D (Couvdat et al., 2012). In a simulation conducted with the CMAQ model over the eastern US, MFB values for  $PM_{2.5}$ , OC and EC were  $-3\%$ ,  $37\%$  and  $14\%$ , respectively (Bailey et al., 2007). Those are lower than the values reported here (Table 4). However, for sulfate a MFB of  $25\%$  reported here is lower in absolute value than the value of  $-35\%$  reported by Bailey et al. (2007).

## 5 Conclusions

A modeling study of meteorology and air pollution in Beirut was conducted for the period of 2–18 July 2011 using WRF and Polyphemus/Polair3D. WRF reproduces satisfactorily the diurnal variations for temperature, wind speed, relative humidity and atmospheric pressure and agrees relatively well with observation of wind direction especially from 6 to 10 July 2011. The WRF results show acceptable performance compared to

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values reported in other studies in Europe and the United States, however, measurements were available for model performance evaluation only at one site. The air quality modeling results in Beirut, show higher  $\text{NO}_2$  concentrations near the coast in the city of Beirut and its northern suburb and lower  $\text{O}_3$  concentrations within the city limits. Highest values for  $\text{PM}_{2.5}$ , OC, and EC are modeled within the city limits suggesting that the major sources which lead to the formation of  $\text{PM}_{2.5}$  are anthropogenic sources. The CTM performance evaluation results show that Polyphemus/Polair3D reproduces satisfactorily  $\text{O}_3$ ,  $\text{PM}_{2.5}$ , OC, EC, and sulfate concentrations. Statistical indicators obtained for the major pollutants are in the range of other studies conducted in Europe and the USA Furthermore, the  $\text{O}_3$  diurnal variation is well reproduced by the model. This modeling study is the first one conducted for Beirut. It provides an overview of the pollutant concentrations in the summer of 2011. Future work should focus on the improvement of the input data such as the emission inventory and the meteorology in order to reduce bias and errors between modeled and observed concentrations. Accordingly, specific emission factors for Lebanon which are not existent up to now are needed as future improvements. These emissions factors could be obtained through measurement campaigns at several point sources. In particular, a measurement campaign in a road tunnel in Beirut is highly recommended in order to obtain specific road transport emission factors representative of the Lebanese fleet. Moreover, the development of a regional emission inventory for the Middle East region would help in reducing biases and errors generated from the boundary conditions due to large uncertainties related to emission inventories in this region. Furthermore, observational data from more than one site typically two or three sites in the city of Beirut are needed to better evaluate the model. In particular, measurements of meteorological variables at many sites are needed to better reproduce the meteorology through data assimilation and measurements of particulate pollutants and gases are needed to evaluate the model accuracy to reproduce these pollutant concentrations in various areas of the study domain.

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Supplementary material related to this article is available online at:  
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acpd-12-29571-2012-supplement.pdf](http://www.atmos-chem-phys-discuss.net/12/29571/2012/acpd-12-29571-2012-supplement.pdf).

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**Table 1.** Numerical options and physical parameterizations considered.

Options	M1	M2	M3	M4	M5
UCM	no	yes	yes	no	no
PBL	YSU	YSU	MYNN	MYNN	YSU
Continuous simulations	yes	yes	yes	yes	no*

\* Restart every two days.

**Table 2.** Statistical performance evaluation of the meteorological variables for the WRF simulations.

Wind speed						
Simulation	RMSE ( $\text{m s}^{-1}$ )	MFB %	MFE %	NMB %	NME %	Correlation
M1	1.34	34	50	43	55	0.74
M2	1.63	39	55	56	66	0.72
M3	1.54	32	56	45	62	0.63
M4	1.33	26	50	33	53	0.63
M5	1.43	35	54	45	60	0.55
Wind direction						
Simulation	RMSE ( $^{\circ}$ )	MFB %	MFE %	NMB %	NME %	Correlation
M1	92.06	23	41	21	35	0.38
M2	93.5	24	41	21	35	0.36
M3	94.23	20	41	19	34	0.39
M4	94.6	20	42	20	35	0.35
M5	132.48	35	62	44	61	0.23
Surface air temperature						
Simulation	RMSE ( $^{\circ}\text{C}$ )	MFB %	MFE %	NMB %	NME %	Correlation
M1	1.54	5	5	5	5	0.9
M2	1.19	4	4	4	4	0.91
M3	0.88	2	3	2	3	0.91
M4	1.18	4	4	4	4	0.91
M5	1.47	3	5	3	5	0.84
Relative humidity						
Simulation	RMSE (%)	MFB %	MFE %	NMB %	NME %	Correlation
M1	12.78	4	12	4	12	0.20
M2	13.46	5	13	5	13	0.14
M3	12.65	8	13	8	13	0.31
M4	12.17	7	12	7	12	0.33
M5	11.62	5	11	5	11	0.21
Atmospheric pressure						
Simulation	RMSE (hPa)	MFB %	MFE %	NMB %	NME %	Correlation
M1	13.83	1	1	1	1	0.98
M2	13.85	1	1	1	1	0.98
M3	14.01	1	1	1	1	0.97
M4	14	1	1	1	1	0.97
M5	13.96	1	1	1	1	0.88

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**Table 3.** Results from simulations A1 to A4 from 2 to 18 July 2011 at USJ.

	O <sub>3</sub> Mean concentration ( $\mu\text{g m}^{-3}$ )	CO Mean concentration ( $\mu\text{g m}^{-3}$ )	NO <sub>x</sub> Mean concentration ( $\mu\text{g m}^{-3}$ )	PM <sub>2.5</sub> Mean concentration ( $\mu\text{g m}^{-3}$ )
Observations at USJ	51	519	65	22
A1	95	703	69	20
A2	136	702	31	22
A3	82	702	72	19
A4	50	703	68	20

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**Table 4.** Statistical performance evaluation for O<sub>3</sub>, NO<sub>2</sub>, NO<sub>x</sub>, CO and some VOC at USJ.

Species	Observed Mean ( $\mu\text{g m}^{-3}$ )	Modeled Mean ( $\mu\text{g m}^{-3}$ )	MFB	MFE	MNB	MNE
O <sub>3</sub> <sup>a</sup>	51	50	−17 %	33 %	−9 %	33 %
NO <sub>x</sub>	65	69	27 %	118 %	74 %	108 %
NO <sub>2</sub>	54	54	16 %	105 %	42 %	76 %
CO	519	703	20 %	41 %	55 %	73 %
TOL	19 <sup>b</sup>	7 <sup>c</sup>	−96 %	97 %	−61 %	62 %
XYL	17 <sup>d</sup>	8 <sup>e</sup>	−87 %	89 %	−55 %	58 %
$\alpha$ -Pinene	0.05	0.1 <sup>f</sup>	37 %	97 %	261 %	301 %
Isoprene	0.62	0.4	−94 %	122 %	−14 %	109 %

<sup>a</sup> A threshold value of 80  $\mu\text{g m}^{-3}$  was used for observations.

<sup>b</sup> The “TOL” measured species include toluene, ethylbenzene, butylbenzene, isopropylbenzene and propylbenzene.

<sup>c</sup> The “TOL” modeled species includes also other minor monosubstituted aromatics.

<sup>d</sup> The “XYL” measured species includes xylene, trimethylbenzene and ethyltoluene.

<sup>e</sup> The “XYL” modeled species includes also other minor polysubstituted aromatics.

<sup>f</sup> The “ $\alpha$ -pinene” modeled species includes  $\alpha$ -pinene and sabinene.

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**Table 5.** Statistical performance evaluation for PM<sub>2.5</sub>, OC, EC and particulate sulfate, nitrate and ammonium at USJ.

Species	Observed Mean ( $\mu\text{g m}^{-3}$ )	Modeled Mean ( $\mu\text{g m}^{-3}$ )	RMSE ( $\mu\text{g m}^{-3}$ )	MFB	MFE
PM <sub>2.5</sub>	21.9	19.93	9.89	−21 %	39 %
OC	5.6	3.24	2.93	−59 %	61 %
EC	1.8	1.17	1.05	−33 %	56 %
Sulfate	6.06	7.35	5.35	25 %	61 %
Nitrate	0.32	0.0049	0.39	−189 %	189 %
Ammonium	1.87	0.32	1.9	−114 %	128 %

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**Fig. 1.** The modeling domains D1, D2 and D3 used in this study.

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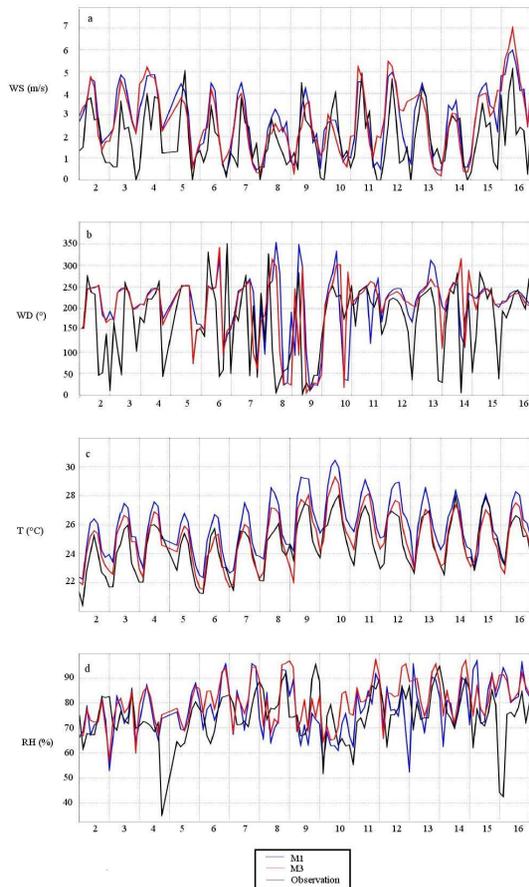
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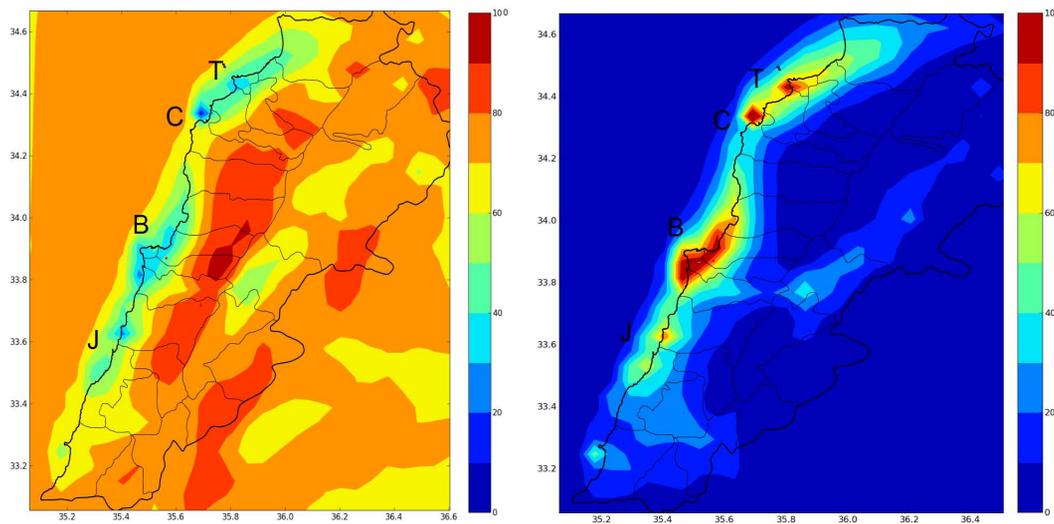




**Fig. 2.** Temporal variation of meteorological variables (observations and model simulations M1 and M3) from 2 till 17 July 2011; **(a)** wind speed ( $\text{m s}^{-1}$ ); **(b)** wind direction ( $^{\circ}$ ); **(c)** air temperature ( $^{\circ}\text{C}$ ); **(d)** relative humidity (%).

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**Fig. 3.** Modeled average  $O_3$  concentrations (left) and  $NO_2$  concentrations (right) in  $\mu g m^{-3}$  for the outer domain D2 (T = Tripoli; C = Chekka; B = Beirut; J = Jieh).

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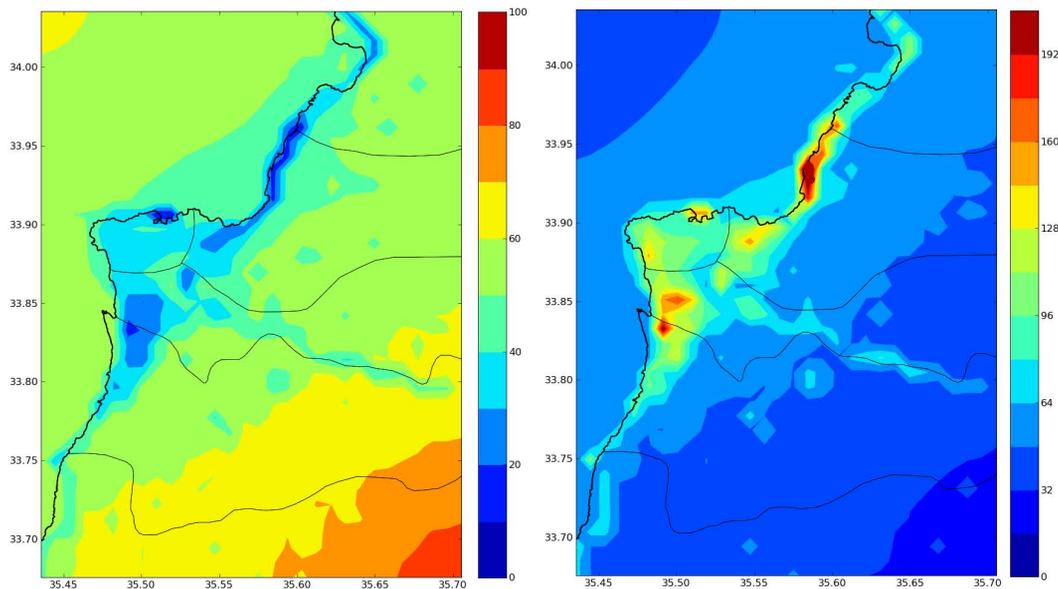
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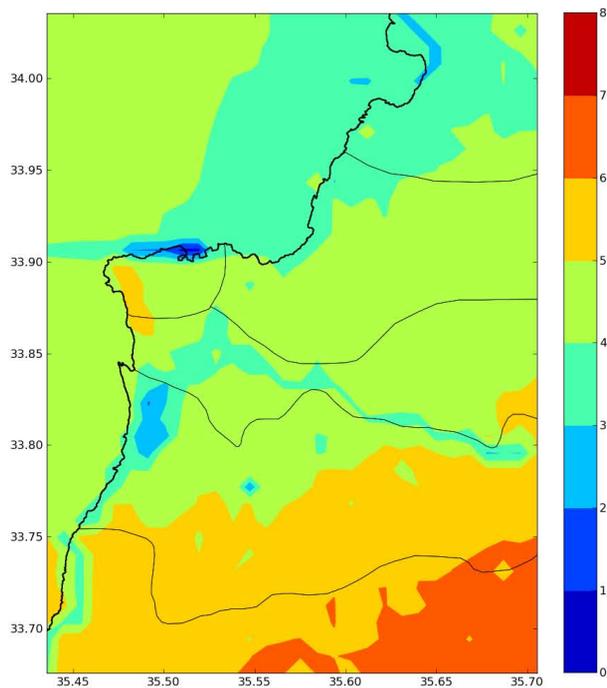


**Fig. 4.** Modeled average O<sub>3</sub> concentrations (left) and NO<sub>2</sub> concentrations (right) in µg m<sup>-3</sup> for the inner domain D1.

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**Fig. 5.** Modeled average VOC/NO<sub>x</sub> ratio for the inner domain D1.

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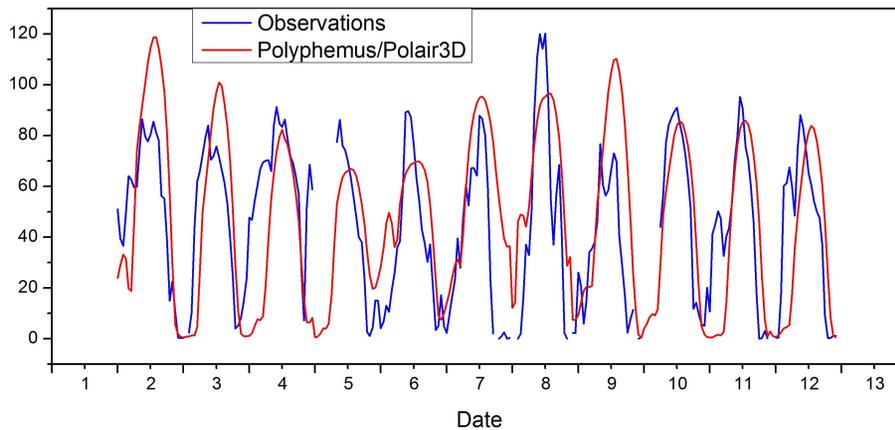
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**Fig. 6.** Temporal variation of observed and modeled  $\text{O}_3$  concentrations in  $\mu\text{g m}^{-3}$  from 2 till 13 July 2011.

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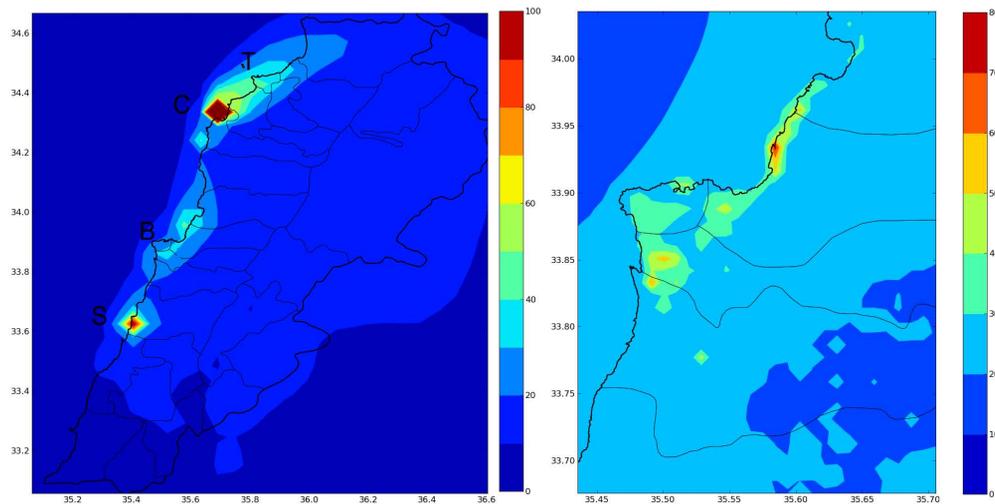
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**Fig. 7.** Modeled average PM<sub>2.5</sub> concentrations in µg m<sup>-3</sup> in Lebanon (left) and in the city of Beirut and its suburbs (right) (T = Tripoli; C = Chekka; B = Beirut; S = Sibline).

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