Application of WRF-Chem model to simulate ozone concentration over Bogota

Anikender Kumar[1], Alexander Rincón[1], Néstor Rojas[1]

[1] Department of Chemical and Environmental Engineering, Universidad Nacional de Colombia, Bogota, Colombia

Corresponding author: Anikender Kumar, anikender@gmail.com

Abstract

The fully coupled WRF-Chem (Weather Research and Forecasting with Chemistry) model is used to simulate air quality over Bogota. Bogota is a tropical South-American megacity located over a plateau in the middle of very complex terrain. An extensive sensitivity analysis to model gas phase chemistry schemes was performed. The WRF-Chem model was adopted for simulating the hourly ozone concentrations for three episodes, representative of dry, intermediate/transition and wet periods in 2010. The computational domains were chosen of 120x120x32, 121x121x32 and 121x121x32 grid points with horizontal resolutions of 27, 9 and 3 respectively. The model was initialized with real boundary conditions using NCAR-NCEP's Final Analysis (FNL) and a 1^{o}x1^{o} (~111 km x 111 km) resolution. Boundary conditions were updated every 6 hours using reanalysis data. The emission rates were obtained from global inventories, namely the REanalysis of the TROpospheric (RETRO) chemical composition and the Emission Database for Global Atmospheric Research (EDGAR). Comparisons between estimated and observed ozone concentrations were carried out through a series of common statistics. In this study, the atmospheric concentrations of ozone over Bogota were calculated to be 40-60 ppb during the simulation periods. Overall, the present case study shows that the model has an acceptable performance over Bogota. This study provides a general overview of WRF-Chem and can constitute a reference for future mesoscale air quality modeling exercises over Bogota and other Colombian cities.

Key words: WRF-Chem, Air Quality Modeling, Ozone, Bogota

1. Introduction

Poor air quality can have an adverse impact on human health including asthma, impaired lung functions, cardiorespiratory illnesses and increased mortality rates, on the ecosystem and on climate Yahya et al., 2014). Air pollution has become one of the most important concerns of the local authorities of Latin American cities and there are many areas where air quality is one of the main environmental issues. So, there is a need for further research to estimate the impact of anthropogenic gas and aerosol emissions on its atmospheric concentrations. Air quality models can be classified into online- and offline-coupled models based on the coupling of meteorology and chemistry. Offline-coupled models use outputs from a meteorological model to drive a chemical transport model and can only simulate the impact of meteorology on chemistry. Online-coupled models allow two-way interactions between the meteorology and chemical constituents through the exchange of meteorological and chemical information at every time step (Zhang, 2008). This paper presents the results of application and evaluation of the 3-D online-coupled Weather Research and Forecasting with Chemistry (WRF-Chem; Grell et al. 2005) model for calculation of meteorological and air pollutants parameters at relatively high spatial resolution at the regional scale. The WRF-Chem simulation was performed with the air quality standards exceeded for ozone in Bogota, capital city of Colombia. There are many reasons for looking particularly at Bogota. First, Bogota is the capital city of Colombia and fifth most populated city in Latin America with around 8.5 million inhabitants. Second, the emissions from traffic are nowadays an increasing concern for the city. Third, the levels of air pollutant concentrations have been shown well above from national air quality standard (NAQS), especially for ozone and particulate matter. The WRF-Chem model results were evaluated with observed measurements collected in the innermost model domain.

2. Model Description and Evaluation

2.1 Episode Selection

The selection of the period for the WRF-Chem simulation is based on the 2010-12 air quality measurements performed on the national air quality network in Bogota, Colombia. The simulations were conducted for eight high ozone episodes of the year 2010; from 01 Jan 00h UTC to 03 Jan 06h UTC, 05 Jan 00h UTC to 07 Jan 06h UTC, 13 Feb 00h UTC to 15 Feb 06h UTC, 27 Feb 00h UTC to 01 Mar 06h UTC, 01 Apr 00h UTC to 03 Apr 06h

UTC, 21 Aug 00h UTC to 23 Aug 06h UTC, 11 Sep 00h UTC to 13 Sep 06h UTC, and 11 Dec 00h UTC to 13 Dec 06h UTC. The selection of temporal domain is based on 8 h maximum O3 exceeding 60 ppb at-least two monitoring stations considering with at-least two consecutive days across the study area. The first 06h of each period is considered as spin-up, while the remaining hours are used for analysis. This approach allows the evaluation of the chemical transport model (CTM) under different atmospheric conditions, which are relevant for air quality.

2.1 WRF-Chem Model Configuration

The model was configured with three two way nested domains with spatial resolution changing from 27km to 3km (Fig. 1). The WRF-Chem model was built over a mother domain (D1) with 27 km spatial resolution of 120 columns and 120 rows, centered at 4.61°N, 74.01°W. It covers Colombia, Ecuador, Venezuela, some part of Pacific Ocean, Atlantic Ocean and Caribbean Sea. The first nested domain (D2) with 9 km spatial resolution of 121 columns and 121 rows, comprises the whole Colombia. The innermost domain (D3) is centered over Cundinamarca area, which include Bogota with 121 columns and 121 rows of 3km x 3km grid cells. Topography, land use and land water datasets are interpolated from USGS with the appropriate spatial resolution of each domain (10', 2', and 30'' for D1, D2 and D3 respectively). The model is initialized by real boundary conditions using NCAR-NCEP's Final Analysis (FNL) data (NCEP-DSSI, 2005) having a spatial resolution of 1° x 1° (~111 km x 111 km) and 6h temporal resolution. The emissions used are based on Emissions Database for Global Atmospheric Research (EDGAR) emission inventory.

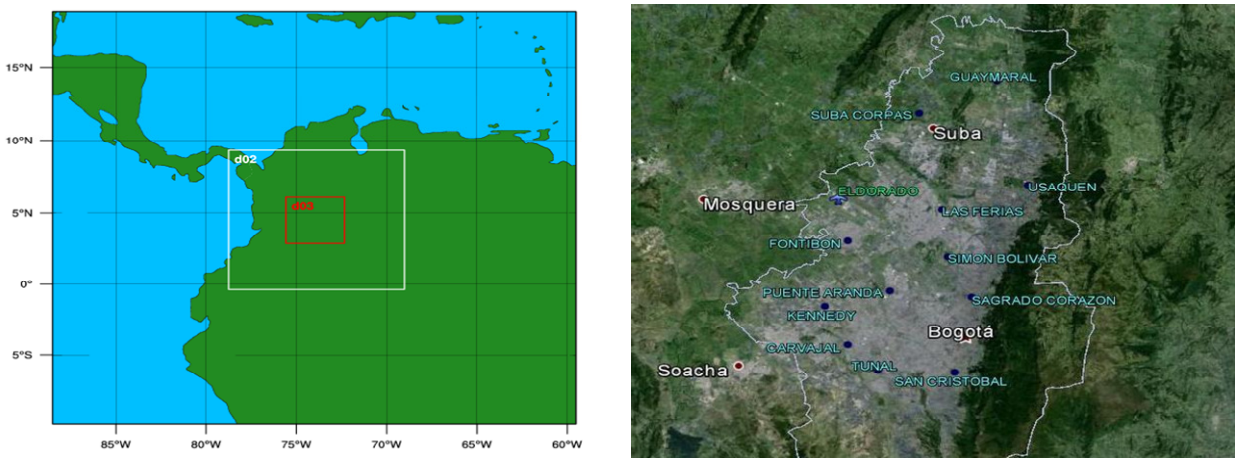


Fig 1: Configuration of the WRF model domains (left) and air quality monitoring stations over the domain d03 during the study period

2.2 Description of Model Physics and Chemistry Options

Number of the physics options for planetary boundary layer (PBL), land surface model (LSM), microphysics, radiation and cumulus parameterizations are available in WRF-Chem model. The common set of parameterizations chosen is the following: Microphysics, Pardue Lin scheme (Lin et al., 1983); long-wave radiation scheme, Rapid and accurate Radiative Transfer Model (RRTM) (Mlawer et al., 1997); and short-wave radiation scheme by Dudhia (1989). Cumulus parameterization schemes are responsible for the subgrid-scale effects of convective and/or shallow clouds but are valid only for coarse-grid sizes such as greater than 10 km. The Kain-Fritsch Scheme (Kain and Fritsch, 1993) is considered for model experiments since this is the most widely exercised option for Cumulus parameterization. The impact of PBL schemes has been addressed on air quality modelling (Mao et al, 2006; Perez et al, 2005). The Yonsei University PBL scheme (YU) (Hong et al., 2006) is a first-order scheme that uses non-local eddy diffusivity coefficients to compute turbulent fluxes. At unstable conditions, local transport is used for subsidence, while upward fluxes are modelled combining local eddy diffusion with a non-local approach that computes the transition probability between non-consecutive levels. LSMs combine atmospheric information from the surface layer scheme with land-surface properties (dependent on land uses) to evaluate the vertical transport done in the PBL schemes, which has a direct influence on the estimation of the PBL height (PBLH) (Han et al., 2008). The Noah LSM (Chen and Dudhia, 2001) scheme is used in the present study. The gas phase chemistry model used is the Regional Acid Deposition Model, version 2 (RADM2) (Stockwell et al., 1990), that includes 57 chemical species and 158 gas phase reactions, of which 21 are photolytic. The aerosol module includes the Modal Aerosol Dynamics Model for

Europe (MADE) (Ackermann et al., 1998) for the inorganic fraction, and the Secondary Organic Aerosol Model (SORGAM) (Schell et al., 2001) for the carbonaceous secondary fraction. MADE/SORGAM in WRF/Chem uses the modal approach with three log-normally distributed modes (nuclei, accumulation and coarse mode).

2.3 Evaluation of the model results

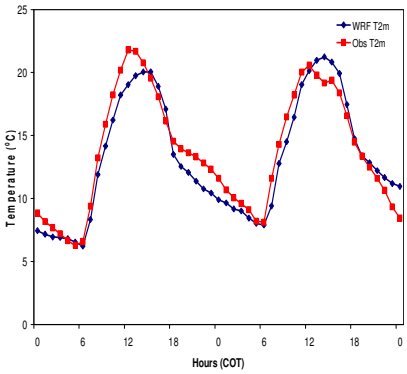
The evaluation of this study is carried out in the focus of the fine-grid domain (D3), since the objective of this study is to assess the sensitivity of the model for high resolution simulations. Fig. 1 shows the location of all the 12 stations namely Carvajal, Fontibon, Guaymaral, Las Ferias, Simon Bolivar, Puente Aranda, Suba Corpas, Tunal, Usaquen, Kennedy, Simon Bolivar, Sagrado Corazon and San Cristobal, selected to provide the surface meteorological observations on hourly basis over Bogota. These meteorological and air pollutants data are provided by Environmental agency of Bogota. There are multiple methodologies available for model evaluation. The selected statistics for the evaluation are taken from Borge et al. (2008), which is specifically developed to evaluate the mesoscale meteorological simulations for air quality purposes. Surface temperature, relative humidity, wind speed, weed direction and ozone were compared and the results summarized using mean bias (MB), gross error (GE), root mean square error (RMSE) and index of agreement (IA) (Willmott, 1982).

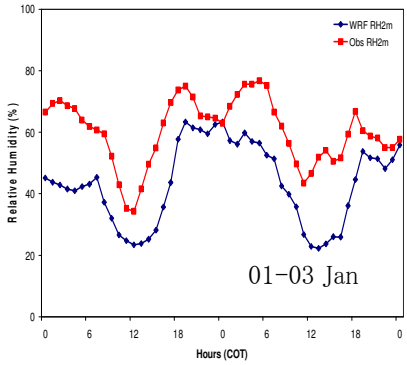
3. Results and Discussions

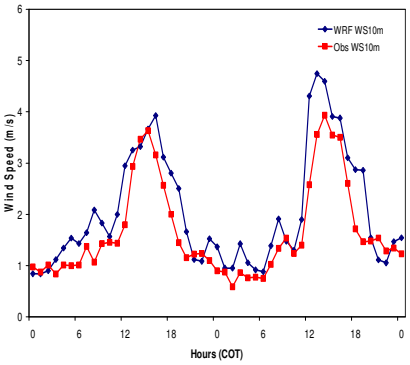
The model is able to correctly resolve temporal changes of surface temp, relative humidity and wind speed with the statistical errors calculated for all measurements (Table 1 and Fig. 2). There is a general tendency of the model to underestimate the observed temp and wind speed for the selected period of ozone episodes, described by the negative MB values. This table shows that the BE, GE and IOA are (-0.32, 1.82, 0.91) and (0.78, 11.94, 0.79) for temperature and relative humidity respectively. In addition, the BE, RMSE and IOA are -0.04, 1.64 and 0.65 for wind speed. There is a general tendency towards under prediction of before noon temperature averages while over prediction for after noon temperatures as suggested in Figure 2. However, there is a consistent under prediction for wind speed in most of the time of all periods. Figure 2 also reveals that there is an overestimation for relative humidity in most of time of all the episodes except the Jan month's periods. The wind direction, being an angular quantity, is compared with wind roses. The hourly average angular distribution of WRF model simulated and observed wind directions at 10 m is shown in the form of wind rose in Figs. 3 (a) and (b), respectively. Both the figures show that both simulated and observed wind directions are prevailing from southeast and southwest directions. The WRF-Chem model simulated 8 hr max Ozone has been compared with observed ozone for all monitored stations in Fig. 3 and it has been found that model is overestimating the max 8 hr Ozone concentration. The Model Simulated concentration of Ozone is shown spatially as Fig. 4 over Bogota and it has been shown that the pollutant is very well distributed spatially in different episodes over the study domain.

Table 1: Error statistics of temperature, wind speed, relative humidity, wind direction and ozone

Variable/Errors	BE	GE	RMSE	IA
T	-0.32	1.82		0.91
WS	-0.04		1.64	0.65
RH	0.78	11.94		0.79
WD	-15.43	94.21		
O3 (max 8 hr)	6.39	17.77	21.46	0.42







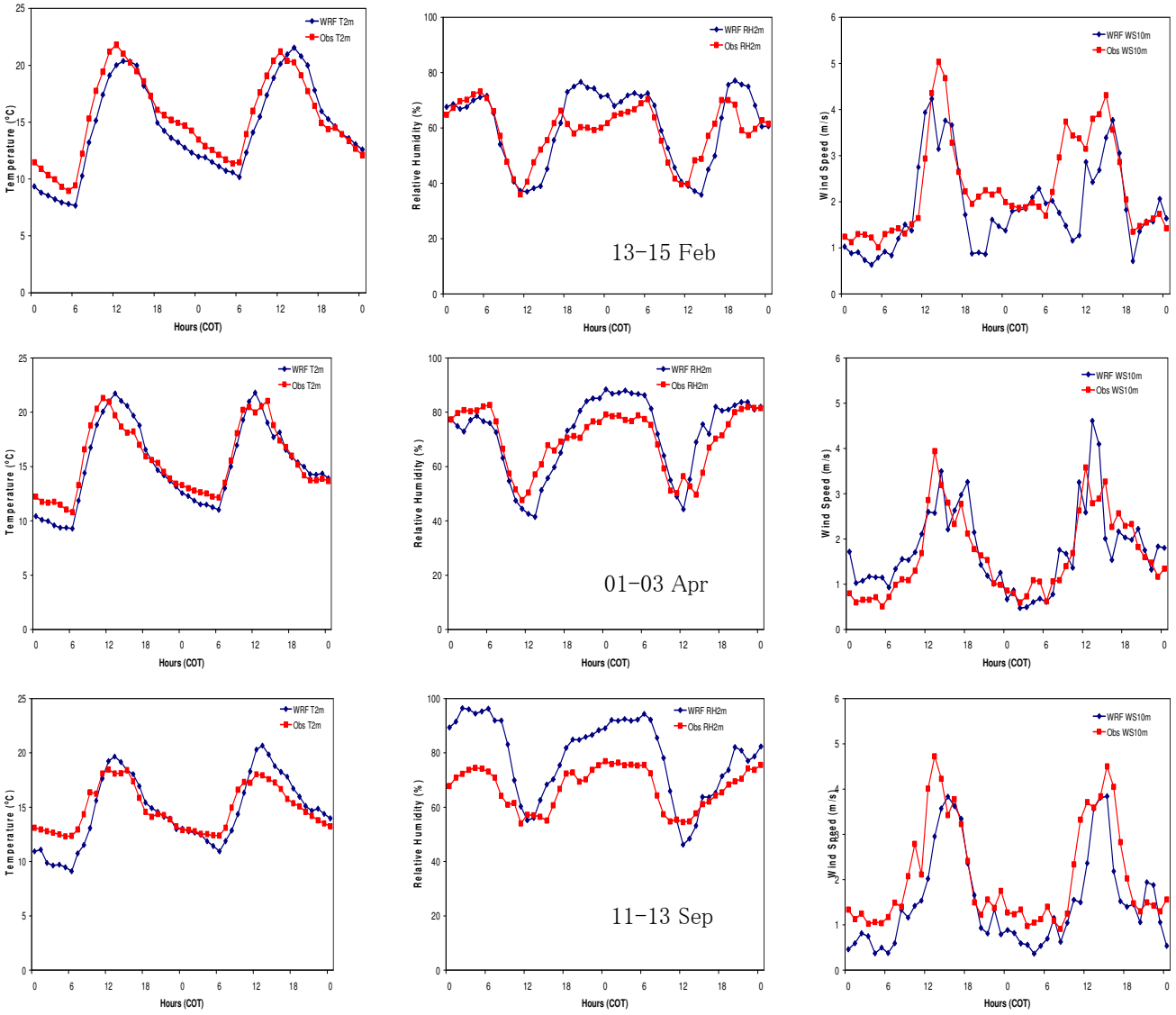


Fig. 2: Comparison of hourly time series between WRF model and observed meteorological parameters temperature (°C), relative humidity (%) and wind speed (m/s) averaged over all the monitoring stations

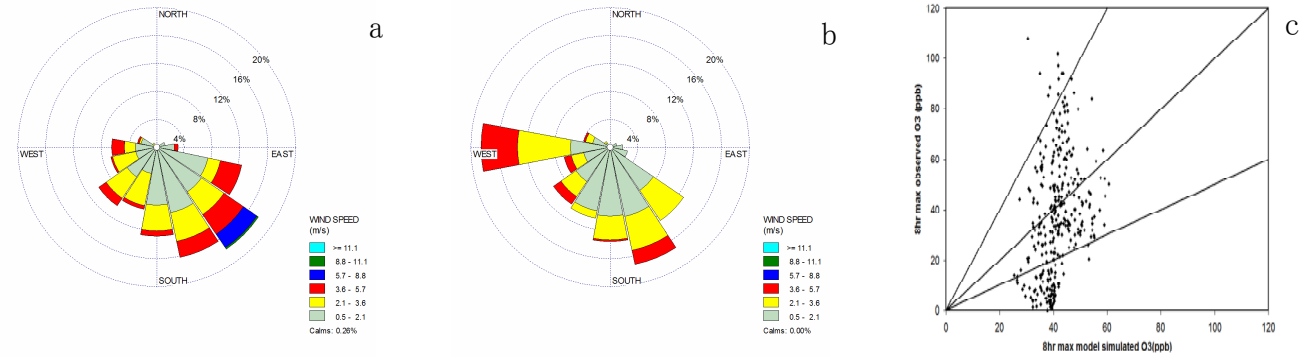


Fig. 3: Comparison of wind rose plots of (a) WRF model (b) observation and (c) comparison between WRF-Chem model and observed 8 hr max Ozone (ppb) during the whole study period over all the monitoring stations

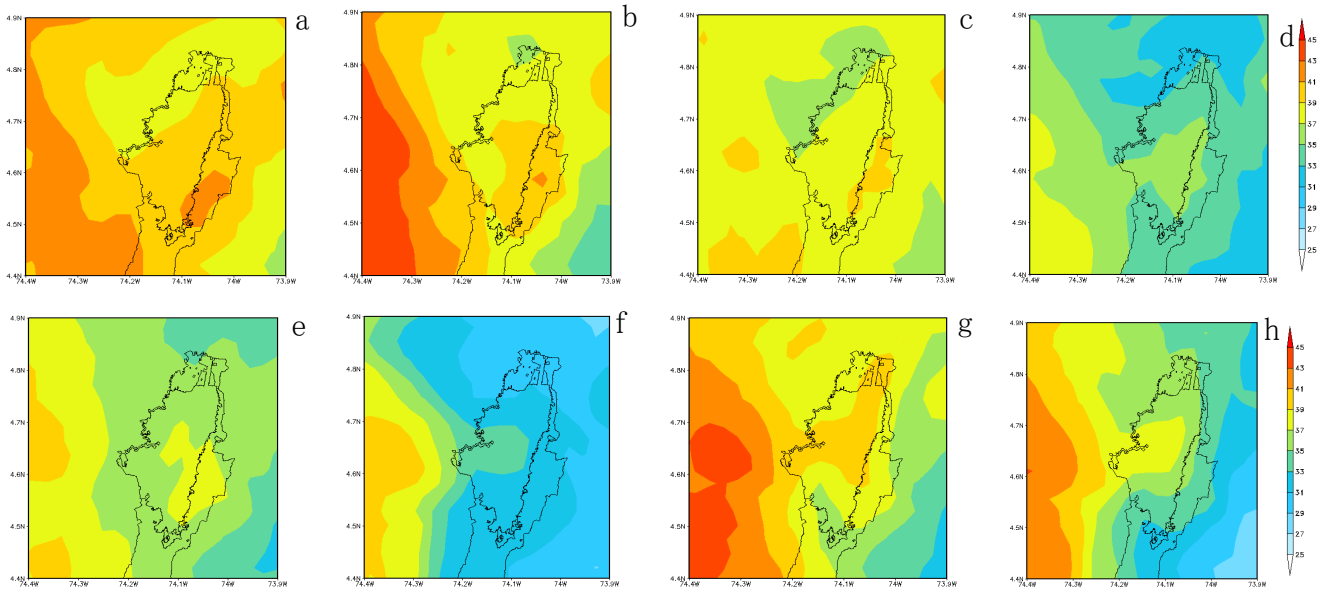


Fig. 4: Spatial Distribution of WRF-Chem model simulated 24h avg Ozone (ppb). These panels (a, b, c, d, e, f, g and h) are 01-02 Jan, 02-03 Jan, 13-14 Feb, 14-15 Feb, 01-02 Apr, 02-03 Apr, 11-12 Sep and 12-13 Sep of year 2010 respectively

4. Summary and conclusions

In this study WRF-Chem model was applied to simulate meteorological and air pollutants parameters over Bogota for the selected period of high concentrations of O3. The main findings are:
The model is capable of reproducing the temporal changes of surface temperature, relative humidity and wind over study area. The model constantly underestimates the measured air temperature and wind speed for selected ozone episodes.
The WRF-Chem model is also overestimating the observed 8h max ozone concentration over study domain for selected episodes. It shows that EDGAR emissions overestimate the pollutants emissions over Colombia. So the use of region emission inventory over Colombia may improve the results of WRF-Chem.

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References

Borge R., Alexandrov V., del Vas J. Jose, Lumbreras J., Rodriguez E., 2008. A comprehensive sensitivity analysis of the WRF model for air quality applications over the Iberian Peninsula. Atmospheric Environment 42, 8560-8574.
Chen E., Dudhia J., 2001. Coupling an advanced land-surface/hydrology model with the Penn State/ NCAR MM5 modeling system. Part I: model description and implementation. Monthly Weather Review 129, 569-585.
Dudhia J., 1989. Numerical study of convection observed during the winter monsoon experiment using a mesoscale two-dimensional model. Journal of Atmospheric Science 46, 3077-3107.
Grell A.G., Peckham S.E., Schmitz R., McKeen S.A., Frost G., Skamarock W.C., Eder B., 2005. Fully coupled “online” chemistry within the WRF model. Atmospheric Environment 39, 6957-6975.
Han Z., Ueda H., An J., 2008. Evaluation and intercomparison of meteorological predictions by five MM5-PBL parameterizations in combination with three land-surface models. Atmospheric Environment 42, 233-249.
Hong S.Y., Noh Y., Dudhia J., 2006: A new vertical diffusion package with an explicit treatment of entrainment processes. Monthly Weather Review 134, 2318–2341.
Kain J.S., Fritsch J.M., 1993. In Convective parameterization for mesoscale models: The Kain-Fritcsh scheme,

The representation of cumulus convection in numerical models, Emanuel K. A. and D.J. Raymond (Eds.), American Meteorological Society, pp. 246.
Lin Y. L., Farley R.D., Orville H.D., 1983. Bulk parameterization of the snowfield in a cloud model. Journal of Climatology and Applied Meteorology 22, 1065–1092.
Mao Q., Gautney L.L, Cook T.M., Jacobs M.E., Smith S.N., Kelsoe J.J., 2006. Numerical experiments on MM5-CMAQ sensitivity to various PBL schemes. Atmospheric Environment 40, 3092-3110.
Mlawer E.J., Taubman S.J., Brown P.D., Iacono M.J., Clough S.A., 1997. Radiative transfer for inhomogeneous atmosphere: RRTM, a validated correlated—k model for long wave. Journal of Geophysical Research 102, 16663–16682.
NCEP-DSS1, 2005. NCEP Global Tropospheric Analyses, (1x1 deg), from Data Support Division (DSS), NCAR, Dataset # 083.2. /http://dss.ucar.edu/datasets/ds083.2/ (accessed June 2005)S.
Perez C., Jimenez 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.
Schell B., Ackermann I. J., Hass H., Binkowski F. S., Ebel A., 2001. Modeling the formation of secondary organic aerosol within a comprehensive air quality model system. Journal of Geophysical Research 106, 28,275–28,293, doi:10.1029/2001JD000384.
Stockwell W. R., Middleton P., Chang J. S., Tang X., 1990. The second generation regional acid deposition model chemical mechanism for regional air quality modeling. Journal of Geophysical Research 95, 16,343–16,367, doi:10.1029/ JD095iD10p16343.
Willmott C., 1982. Some comments on the evaluation of model performance. Bulletin of American Meteorological Society 63, 1309-1313.
Yahya K., Wang K., Gudoshava M., Glotfelty T., Zhang Y., 2014. Application of WRF/Chem over North America under the AQMEII Phase 2: Part I. Comprehensive Evaluation of 2006 Simulation. Atmospheric Environment, doi: 10.1016/j.atmosenv.2014.08.063.
Zhang Y., 2008. Online-coupled meteorology and chemistry models: history, current status, and outlook. Atmospheric Chemistry and Physics 8, 2895-2932.