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THE NMMB/BSC-CTM: A MULTISCALE ONLINE CHEMICAL WEATHER PREDICTION SYSTEM

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Abstract: The model NMMB/BSC-CTM is a new fully on-line chemical weather prediction system under development at the Earth Sciences Department of the Barcelona Supercomputing Center in collaboration with several research institutions. The basis of the development is the NCEP new global/regional Nonhydrostatic Multiscale Model on the B grid (NMMB). Its unified nonhydrostatic dynamical core allows regional and global simulations and forecasts. A mineral dust module has been coupled within the NMMB. The new system, NMMB/BSC-DUST, simulates the atmospheric life cycle of the eroded desert dust. The main characteristics are its on-line coupling of the dust scheme with the meteorological driver, the wide range of applications from meso to global scales, and the dust shortwave and longwave radiative feedbacks on meteorology. In order to complement such development, the BSC works also in the implementation of a fully on-line gas-phase chemical mechanism. Chemical species are advected and mixed at the corresponding time steps of the meteorological tracers using the same numerical scheme of the NMMB. Advection is Eulerian, positive definite and monotone. The final objective of the work is to develop a fully chemical weather prediction system, namely NMMB/BSC-CTM, able to resolve gas-aerosol-meteorology interactions from global to local scales. Future efforts will be oriented to incorporate a multi-component aerosol module within the system with the aim to solve the life-cycle of relevant aerosols at global scale (dust, sea salt, sulfate, black carbon and organic carbon). In the present contribution we describe the status of development of the system and first evaluation results of the gas-phase chemistry.

Key words: *Atmospheric modeling, Air quality, online models, multiscale.*

INTRODUCTION
The NMMB/BSC Chemical Transport Model (NMMB/BSC-CTM) is a new chemical weather prediction system for short term forecast, currently under development at the Barcelona Supercomputing Center – Centro Nacional de Supercomputación (BSC) in collaboration with several research institutions. The model is able to simulate the tropospheric gas-phase photochemistry (Jorba et al., 2011) and includes the dust processes of NMMB/BSC-DUST (Pérez et al., 2011). The meteorological core of the model is the new NMMB (Janjic, 2005; Janjic and Black, 2007), an evolution of the NCEP operational WRF-NMM model. Gas-phase photochemistry, dust processes, and meteorology are on-line coupled in order to incorporate feedback interactions, such as direct radiative effect and photolysis feedback. In this contribution, the main characteristics of NMMB/BSC-CTM are described and results of the evaluation of the gas-phase chemistry are presented. Future work and plans with the model are discussed in the last section of the manuscript.

MODEL DESCRIPTION
The NMMB/BSC-CTM is based on the atmospheric driver NMMB, and it incorporates a gas-phase chemistry module to solve the tropospheric chemistry and an aerosol module that considers the most relevant aerosols at global scale (e.g., mineral dust, sea salt, black carbon, organic carbon and sulfate). From all the aerosols, the mineral dust scheme is inherited from the NMMB/BSC-Dust model (Pérez et al., 2011). In this section, a brief description of the model components is presented.

Atmospheric driver
The Nonhydrostatic Multiscale Model on the B grid (NMMB; Janjic, 2005; Janjic and Black, 2007; Janjic et al, 2011) is the new unified atmospheric model developed at the National Centers for Environmental Prediction (NCEP) for a broad range of spatial and temporal scales. Its unified nonhydrostatic dynamical core allows regional and global simulations. It evolves from the operational regional WRF-NMM model. The regional NMMB is planned to become operational at NCEP as the regional North American Mesoscale (NAM) model shortly.

Isotropic horizontal finite volume differencing is employed so a variety of basic and derived dynamical and quadratic quantities are conserved (e.g., energy, enstrophy). In the vertical, the hybrid pressure-sigma coordinate is used. The forward-backward scheme is used for horizontally propagating fast waves, and an implicit scheme is used for vertically propagating sound waves. The Adams-Bashforth scheme is applied for horizontal advection of the basic dynamical variables and for the Coriolis force. In order to eliminate stability problems due to thin vertical layers, the implicit Crank-Nicholson scheme is used to compute the vertical advection tendencies. Advection of passive tracers is Eulerian, positive definite and monotone.

The unified dynamical core of the model is developed for the scales ranging from large eddy simulations (LES) to global runs (Janjic, 2005). The global model is constructed in the latitude-longitude grid with polar filtering. In contrast to the WRF-NMM, which is defined on the Arakawa E grid, the dynamics of the NMMB are reformulated for the Arakawa B grid. The nonhydrostatic component of the model dynamics is introduced through an add-on module that can be turned on or off depending on resolution. Across the pole polar boundary conditions are specified in the global limit. In regional applications the rotated longitude-latitude system is used. With the Equator of the rotated system running through the middle of the integration domain, more uniform grid distances are obtained.

The physical package used is composed by the Mellor-Yamada-Janjic (MYJ) level 2.5 planetary boundary layer (PBL) parameterization, the surface layer scheme based on the Monin-Obukhov similarity theory with viscous sublayer over land

and water, the NCEP NOAH or LISS land surface model, the GFDL or RRTM longwave and shortwave radiation package, the Ferrier microphyisics, and the Betts-Miller-Janjic convection parameterization. Trace gases and aerosols can be coupled with the RRTM radiative package through climatological profiles or the aerosol and gas NMMB/BSC-CTM model results. The reader is referred to Janjic et al. (2011) and Pérez et al. (2011) for a further description of the model.

Aerosol module

An aerosol module for the relevant global aerosols (e.g., mineral dust, sea salt, black carbon, organic carbon and sulfate) is under development within the NMMB/BSC-CTM. All mineral dust processes are fully in-lined within NMMB, and an extensive description and evaluation of the dust implementation is presented in Pérez et al. (2011). The sea salt, black carbon, organic carbon and sulfates are currently under development. A brief description of the dust scheme is included below. The Dust module solves the conservation equation for dust taking into account the following processes: 1) dust generation by surface wind and turbulence, (2) horizontal and vertical advection, (3) horizontal diffusion and vertical transport by turbulence and convection (4) dry deposition and gravitational settling and (4) wet removal which includes in-cloud and below-cloud scavenging from convective and stratiform clouds. Advection and diffusion of mineral dust follows the same approach as moisture transport in NMMB. The model includes 8 dust size bins; within each transport bin, dust is assumed to have time-invariant, subbin lognormal distribution. The submicron particles correspond to the clay-originated aerosol (bins 1-4) and the remaining particles to the silt (bins 5-8).

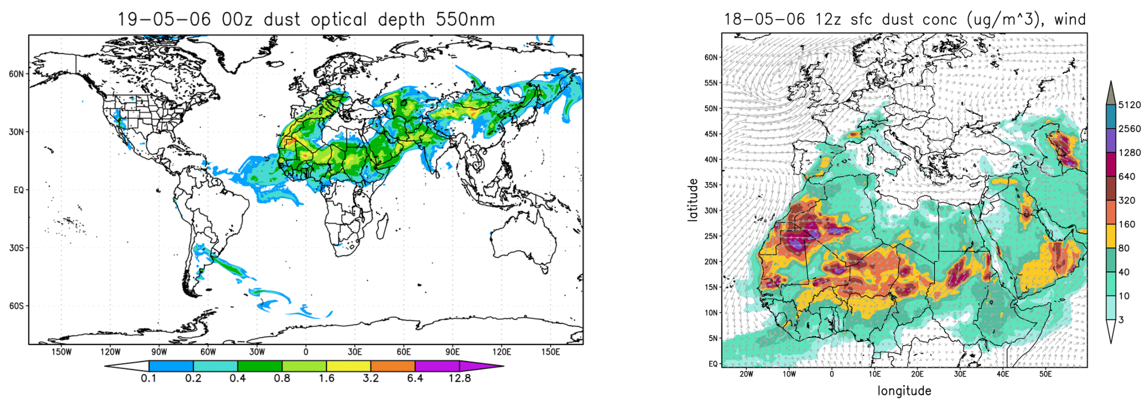

Figure 1. NMMB/BSC-CTM Dust optical depth over the globe (left) and surface concentration at regional scale (right).

The dust emission scheme takes into account the effects of saltation and sandblasting, soil moisture and viscous diffusion close to the ground. It is a function of surface wind speed and turbulence, land use type, vegetation cover, erodibility, surface roughness, soil texture and soil moisture. The emission scheme considers all topographic lows with bare ground surface as preferential sources for dust emission following Ginoux et al. (2001) approach. The seasonal changes in vegetation are considered from a global monthly climatological vegetation fraction estimate from AVHRR. Four top soil texture classes (coarse sand, fine/medium sand, silt, clay) are introduced, based on the new STASGO-FAO 1km soil database.

The dry deposition scheme accounts for the effects of sedimentation and turbulent mixout. In-cloud and below-cloud wet scavenging is considered for grid-scale and convective precipitation. The effect of convection on the dust concentration is parameterized assuming that the relative pattern of dust vertical redistribution is analogous to that of specific humidity after moist convective adjustment. Dust shortwave and longwave radiative feedbacks on meteorology are fully taken into account through the coupling of dust aerosols with the RRTM SW/LW radiation scheme of NMMB (Pérez et al 2006, 2011).

Gas-phase chemistry module

A gas-phase module is implemented within NMMB/BSC-CTM to properly simulate the tropospheric gas-phase chemistry. The tropospheric mechanism is coupled with a simplified linear scheme for the stratospheric chemistry of O_3. Thus, a fully consistent balance in O_3 concentrations is achieved within the troposphere. The modular structure of the system allows configuring the model with feedbacks among the different processes implemented (e.g., radiation-aerosols-gases, photolysis-gases-aerosols). In this section a brief description of the gas-phase chemistry module is presented.

Chemical species are advected and mixed at the corresponding time steps of NMMB tracers using the same numerical scheme as NMMB (Eulerian, positive definite and monotone). The chemical mechanism and chemistry solver is based on the Kinetic PreProcessor KPP package with the main purpose of maintaining a wide flexibility when configuring the model. Two Carbon Bond family chemical mechanism have already been implemented, CB-IV and CB05. Additionally, an Euler-Backward-Iterative solver is implemented to solve the CB05 chemical mechanism. The latter allows configuring the model with an efficient and fast ODE solver. The photolysis scheme is based on the Fast-J scheme, coupled with physics of each model layer (e.g., aerosols, clouds, absorbers as ozone) and it considers grid-scale clouds from the atmospheric driver. The Fast-J scheme has been upgraded with CB05 photolytic reactions.

An emission process allows the coupling of a vast variety of emission inventory sources (e.g., POET, RETRO, EDGAR, MACC, EMEP, HERMES) with the model. Anthropogenic emissions are incorporated from state-of-the-art emission inventories, while natural emissions are computed on-line. Currently, only biogenic emissions are implemented through the coupling of the MEGAN model within NMMB/BSC-CTM.

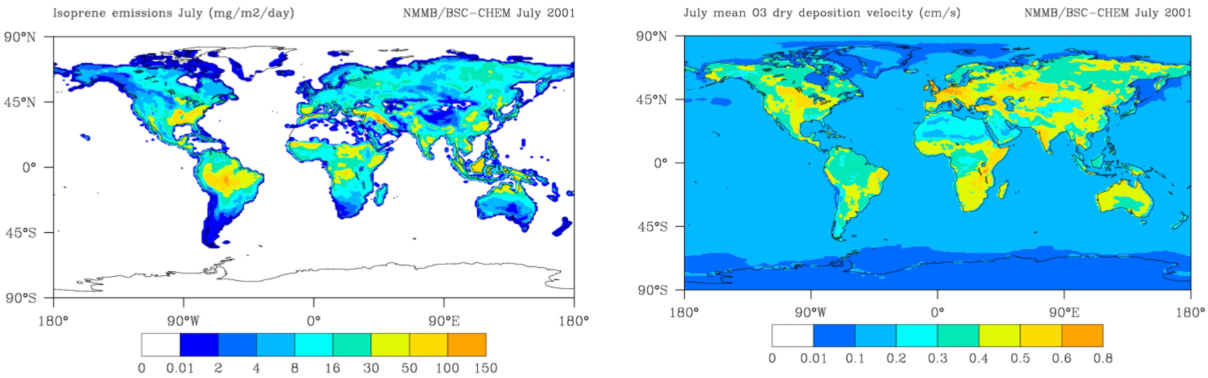

Figure 2. Isoprene emissions computed with NMMB/BSC-CTM (left) and July 2001 mean O_3 dry deposition velocity (right).

The dry deposition scheme follows the deposition velocity analogy for gases, enabling the calculation of deposition fluxes from airborne concentrations. The Wesley scheme is implemented to compute the canopy resistance in the dry-deposition process. The cloud-chemistry processes are included in the system considering both sub-grid and grid-scale processes following Byun and Ching (1999) and Foley et al. (2010). The processes included are the scavenging, vertical mixing and wet-deposition. Only incloud scavenging is considered in the current implementation.

A linear ozone photochemistry parameterization for use in upper troposphere and stratosphere (Cariolle and Teyssedre, 2007) is implemented within NMMB/BSC-CTM. The linear model computes the production-loss trends of O_3 in the upper troposphere and lower stratosphere from the atmospheric temperature, O_3 concentrations, total stratospheric chlorine content and climatological conditions. It provides an accurate approximation about the evolution of the O_3 cycle in the upper atmosphere. The coupling of the linear model with the tropospheric chemical mechanism allows a better balance on the O_3 chemistry within the troposphere. Such an approach is a computationally efficient procedure to take into account the stratosphere-troposphere exchange processes.

EVALUATION RESULTS

The mineral dust module has been extensively evaluated at global and regional scales on an annual basis. Pérez et al. (2011) and Haustein et al. (2011, in preparation) present the evaluations for the mineral dust module. Thus, in this section we focus on the preliminary evaluation results of the gas-phase chemistry of NMMB/BSC-CTM configured at global scale. A global domain at 1.4ºx1º and 64 vertical layers is used. The top of the domain is at 0 hPa. NCEP/Final Analyses (FNL) are used as meteorological initial conditions. The meteorology is restarted each day. To initialize the chemistry, initial conditions from the LMDz-INCA model (Hauglustaine et al., 2004) are used and a spin-up of 6 months is run. The model results are evaluated against ground level observations of O_3, NO_2 and CO. Background stations from the World Data Centre for Greenhouse Gases (WDCG), the Co-operative Programme for Monitoring and Evaluation of the Long-range Transmission of Air Pollutants in Europe (EMEP) and the Clean Air Status and Trends Network in USA (CASTNET) are selected. Furthermore, the vertical structure of O_3 is compared against the available ozonesounds of the World Ozone and Ultraviolet Radiation Data Center ozonesound network (WOUDC). Finally, an independent run is performed to evaluate the preliminary results of the stratospheric linear model coupled with the NMMB/BCS-CTM. No tropospheric chemistry is tuned on for that run. The model is configured at 2.8ºx2º and 64 vertical layers.

Ground level evaluation

The RMSE, MB, MNBE, MNGE, MFB and MFE are computed for July and August 2004. A two-monthly mean is computed. A summary of the results is presented in Table 1. Figure 3 shows the RMSE for stations below 1000m a.s.l. spatially distributed over the USA from CASTNET network, and the global domain from WDCG and EMEP networks. The model presents some underestimation of O_3 and NO_2 at the ground level. The best performance of the system is produced over the USA. Statistics computed with CASTNET stations show a MNGE of 22.67% and a MNBE of 11.5%. There is a clear relation between stations that are located in elevated areas and poor skill of the model. The model shows good results over flat areas (east USA, Asia and Europe coastal stations). Most of those stations located below 1000 m a.s.l. have a RMSE below 8 ppbv. The model also shows a good performance on the background O_3 levels in the Southern Hemisphere, where the RMSE is maintained below 6 ppbv. Considering that we are evaluating a global model at a rather coarse resolution, the statistics obtained are satisfactory. This preliminary evaluation will be complemented with more stations over areas where we do not have observations yet and extended through an annual time scale.

Table 1. Ground level evaluation for July and August 2004.

GAS	Network	Num stns	Obs. Mean	Sim. Mean	MB (ppbv)	RMSE (ppbv)	MNBE (%)	MNGE (%)	MFB (%)	MFE (%)
O_3	WDCGG	41	31.69	27.35	-4.34	11.2	-7.87	25.49	-13.45	26.83
	EMEP	70	38.25	27.25	-11	15.77	24.22	30.38	32.21	37.5
	CASTNET	63	31.73	33.86	2.37	2.21	11.57	22.67	7.58	20.56
NO_2	WDCGG	12	1.94	1.23	-0.71	2.04	29.37	102.26	-30.49	80.74
	EMEP	21	3.9	1.8	-2.1	3.36	-38.85	56.58	-64.45	77.2
CO	WDCGG	14	121.51	145.32	23.82	51.51	43.28	50.14	22.06	29.93

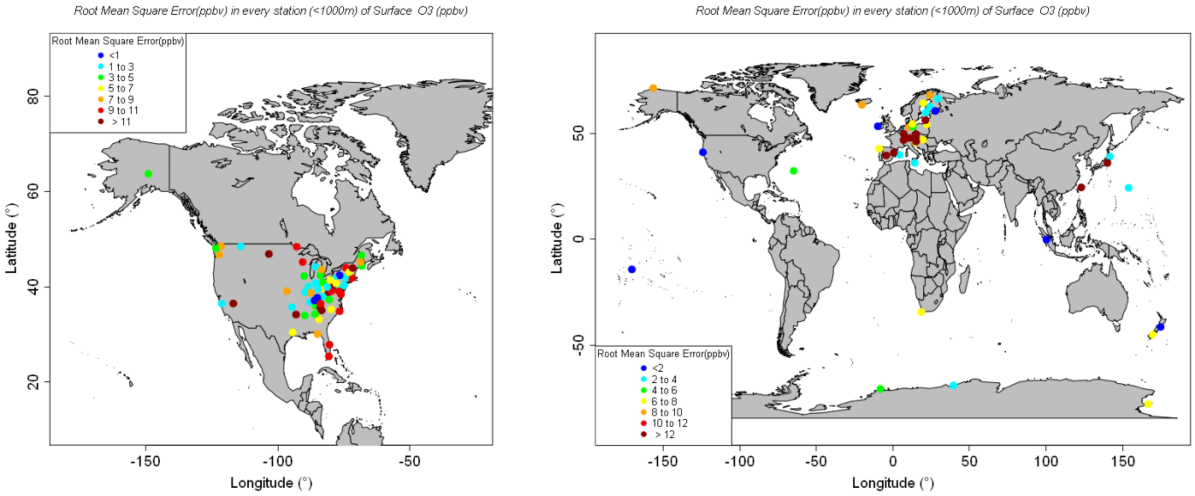

Figure 3. Mean O_3 RMSE (ppbv) at ground level for stations of CASTNET (left), and WDCGG and EMEP (right) networks.

Ozonesondes

The vertical structure of the simulated O_3 has been evaluated with available ozonesondes for July and August 2004. Thus, the RMSE of vertical O_3 is computed adding the error on each vertical level where we have observation and applying the root mean square over the total sum. The total RMSE is plotted in Figure 4, where the location of the available ozonesondes is displayed with the error value. The Northern Hemisphere ozonesondes present errors between 18 and 36 ppbv. There is a systematic underestimation of the O_3 concentration through the troposphere (not shown). The model reproduces reasonably well the vertical structure in the lower and middle troposphere despite the general underestimation. In the upper-troposphere lower-stratosphere, the model presents larger deviations from the observations. That is normal, considering that no special treatment of the upper-troposphere is applied on this simulation. In regards to the performance of the model in the Southern Hemisphere, the RMSE remains below 18 ppbv in most of the locations. Overall, the model performance is reasonably good. The inclusion of a better upper-troposphere chemical condition may improve the present results and reduce the negative bias observed across the whole troposphere.

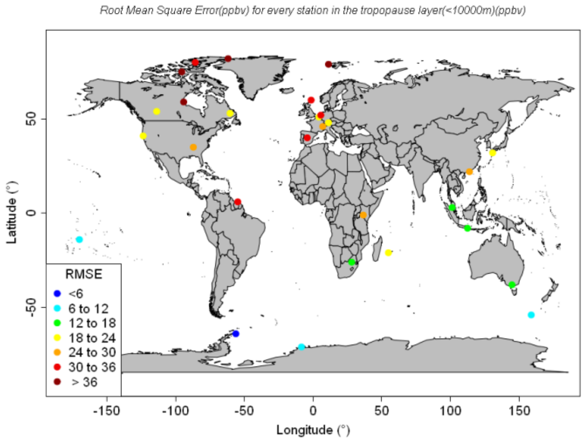

Figure 4. Mean O_3 RMSE (ppbv) at available ozonesonde locations for July and August 2004. Only measurements below 10000 m a.s.l. are considered.

Stratospheric ozone: integrated total ozone column

A specific model configuration has been run to assess the implementation of the stratospheric linear chemistry of O_3 within NMMB/BSC-CTM. Figure 5 shows the total ozone computed with NMMB/BSC-CTM and observed by TOMS satellite. Results for 1 May 2004 and 1 October 2004 are presented. The general structure of the O_3 concentrations is well reproduced by the model. Some general underestimation is observed in equatorial latitudes. Maximum concentrations reported in the Northern Hemisphere are reasonably well captured by the system. In October, the model reproduces the development of the ozone hole over the Antarctica. However, the strength of the hole is underestimated. The distribution over the Southern Hemisphere is well captured and some overestimations are detected over higher latitudes of the Northern Hemisphere. Although those are preliminary results, the model is able to reproduce the major structures observed by TOMS satellite. It is believed that the results may improve after a complete spin-up of one year and a higher resolution configuration.

FUTURE WORK

The future work for the development of the model is structured in several efforts. It is planned to improve and upgrade the numerics and physics of the tropospheric chemistry: gas-phase, dry deposition, cloud chemistry, aqueous-phase chemistry, linear stratospheric chemistry, etc. Furthermore, the aerosol module is currently complemented with the implementation of the other global relevant aerosol species, i.e. sea-salt, black carbon, organic carbon, and sulfate, in addition to dust. Several aerosol processes for sea-salt, black and organic carbon and sulfates will be implemented in the model such as physically-based emissions, water-uptake, dry and wet removal, convective mixing, sulfur chemistry, etc. Additionally, in order to consider feedback processes, it is planned to couple the radiative scheme of NMMB with all the considered aerosol species to simulate the aerosol radiative effect following Pérez et al. (2006) and Pérez et al. (2011). The coupling of the predicted O_3 with the radiative scheme is envisaged. And finally, the coupling of the photolysis scheme with the model aerosol species and O_3 is planned. Overall, extensive evaluation works are planned to qualitatively and quantitatively evaluate the model on global configurations and regional and local runs.

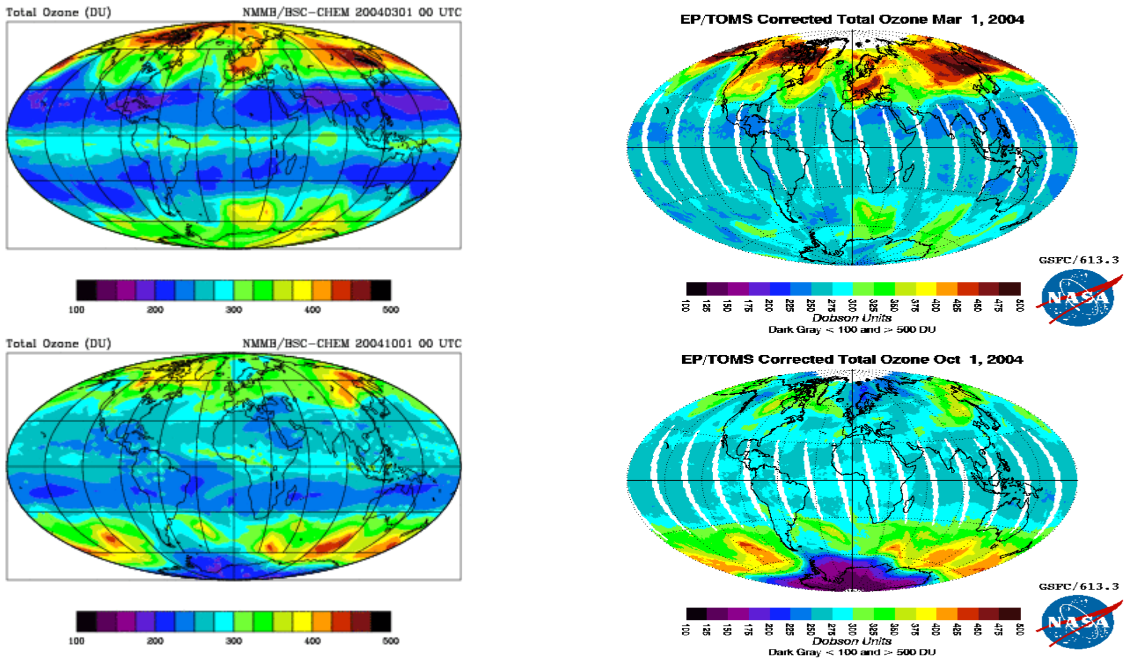

Figure 5. Total Ozone column (DU) modeled by NMMB/BSC-CTM (left) and observed by TOMS (right) for 1 March 2004 (up) and 1 October 2004 (bottom).

CONCLUSIONS

The NMMB/BSC-CTM model is a new state-of-the-art chemical weather prediction system intended to be a powerful tool for air quality tropospheric studies from global to sub-synoptic scales. The NMMB/BSC-CTM configured with the mineral dust module turned on is expected to start providing pre-operational dust forecasts both at global and regional scale within the Sand and Dust Storm-Warning Assessment System (http://sds-was.aemet.es/). The evaluation of the gas-phase chemistry will be complemented on an annual basis at both global and regional scales.

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