

The NMMB/BSC-CTM: a multiscale online chemical weather prediction system

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14th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes

Kos Island, Greece, 2-6 October 2011

BSC air quality modeling activities

CALIOPE daily experimental forecast and verification

Daily experimental forecasts for meteorology and air quality (12 km for Europe and 4 km for the \checkmark Iberian Peninsula) (<u>http://www.bsc.es/caliope</u>).



BSC-DREAM8b daily forecast and verification

North Africa/Mediterranean - 1/3 x 1/3 degree resolution Asia domain - 1/2 x 1/2 degree resolution







→ http://www.bsc.es/projects/earthscience/DREAM



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- Memorandum of understanding NCEP BSC on the use and development of air quality and meteorological modules within the new NMMB NWP model
- Funded by national research projects:
 - Improvement of the Dust Regional Atmospheric Model (BSC-DREAM8b) for prediction of Saharan dust events in the Mediterranean and the Canary Islands [CICYT CGL2006-11879].
 - Coupling of a fully online chemical mechanism within the atmosperic global-regional umo/dream model [CICYT CGL2008-02818].
 - Coupling of a fully online multi-component aerosol module within the atmosperic global-regional NMMB model [CICYT CGL2010-19652].
- Development under a collaborative framework with several research institutions
- Experimental research regional and global air quality modelling system



NMMB/BSC-Chemical Transport Model

Embedding dust and chemistry processes within the meteorological core driver NMMB





BSC

Supercomputing Center

NMMB – Nonhydrostatic Multiscale Model on the B grid – Main characteristics Under development at NCEP (Janjic, 2005; Janjic, 2007; Janjic, 2009)

Unified nonhydrostatic dynamical core (list of features is not exhaustive)

- ✓ Wide range of spatial and temporal scales (from meso to global)
- Regional and global domains (just a simple switch)
- Evolutionary approach, built on NWP experience by relaxing hydrostatic approximation
 Favorable features of the hydrostatic formulation preserved
- ✓ The nonhydrostatic option as an add–on nonhydrostatic module
- ✓ No problems with weak stability on mesoscales
- ✓ Conservation of important properties of the continuous system
- Arakawa B grid (in contrast to the WRF-NMM E grid)
- ✓ Pressure-sigma hybrid
- ✓ Improved tracer advection: Eulerian, positive definite, mass conservative and monotonic

✓ NMMB regional will become the next-generation NCEP mesoscale model for operational weather forecasting in 2011



NMMB/BSC-DUST: a new online mineral dust model

- Evolution of the BSC-DREAM8b model [Nickovic et al., 2001; Pérez et al., 2006]
- NMMB introduction
 - The NCEP-ETA weather forecast model is replaced by a state-of-theart regional/global NWP model with improved dynamics and physics:

→ NCEP-NMMB [Janjic, 2005, 2007, 2009, 2010, 2011]

- New NMMB/BSC-Dust model [Pérez et al., 2008,2011; Haustein et al., 2011]
 - Implementation of all common **on-line dust modules** for global and regional simulations
 - Nested regional domains at very high resolution are available
 - The current DREAM dust emission scheme is upgraded to a physically based scheme → explicitly accounting for saltation and sandblasting
 - New high resolution database for soil textures and vegetation fraction is included
 - Dust direct radiative effect implemented



NMMB/BSC-CTM: gas-phase chemistry

- Implementing the gas-phase chemistry within NMMB/BSC-DUST model.
- Fully on-line modeling system
- NEW NMMB/BSC-CTM [Jorba et al., 2009, 2010, 2011]
 - Wide range of application from global to sub-synoptic scales.
 - Modular implementation within NMMB. Chemistry solved after NMMB physics with the same timestep.
 - The advection, horizontal and vertical diffusion solved using the NMMB numerical schemes.
 - Dust processes of NMMB/BSC-DUST included and feedback interactions allowed.
 - Several gas-phase processes implemented, such as on-line natural emissions from MEGAN model, transport, dry deposition, clouds scavenging and wet deposition.



Tropospheric gas-phase chemistry processes (Jorba et al., 2009-2011; Badia and Jorba, 2011)



- On-line Fast-J scheme (Wild et al., 2000)
- Coupled with physics of each model layer (e.g., aerosols, clouds). Planned to couple with NMMb/BSC-DUST aerosols.
- Considers NMMB grid-scale clouds and NMMB/BSC-CHEM O3 or climatology
- 7 bins wave-length (quick version)

$$J_{i} = \int_{\lambda_{1}}^{\lambda_{2}} F(\lambda) \sigma_{i}(\lambda) \phi_{i}(\lambda) d\lambda$$

 $F(\lambda)$: actinic flux

 $\sigma_i(\lambda)$: absorption cross section

 $\Phi_i(\lambda)$: quantum yield of phot. react.

• Tables of $\sigma_i(\lambda)$ and $\Phi_i\left(\lambda\right)$ to be updated from Prather Fast-JX.

Dry deposition

- Wesely et al. (1986, 1989) implemented to compute deposition velocities
- Simple scheme coupled with surface model layer physics (e.g., skin temperature, incoming shortwave radiation, friction velocity, ...)
- Solve dry deposition in chemistry module independently from vertical diffusion. Considering to solve dry depositoin and vertical diffusion at first model level at same time.

$$\frac{dC_i(z_{ref})/dt = -V_i(z_{ref}) \times C_i(z_{ref})/\Delta z}{V_d = (R_a + R_b + R_c)^{-1}}$$

Chemical mechanism

- CBM-IV and CB05 mechanisms implemented (Gery et al., 1989; Yarwood, 2005)
- Coupled with Fast-J photolysis scheme
- Mechanism implemented through KPP kinetic preprocesor (Damian et al., 2002)
- KPP coupling allows a straightforward modification of chemistry kinetics and reactions. Suitable for sensitivity studies.
- Implemented an EBI solver for CB05

Cloud chemistry

- Cloud chemistry includes: scavenging, mixing, wet deposition and aqueous chemistry
- Scavenging and wet deposition implemented for gridscale and sub-gridscale clouds following Byun and Ching (1999)
 - Sub-grid + gridscale:
- Scavenging:



• Wet deposition:

$$wdep_i = \int_{0}^{\tau_{cld}} \overline{m}_i^{cld} P_r d$$





Stratospheric ozone chemistry

- Proper treatment of STE, improve the balance of tropospheric ozone and specify upper boundary condition for tropospheric ozone
- Implementation of the Cariolle and Teyssèdre (2007) linear model from the tropopause to the model top

$$dr_{O_3}/dt = A_1 + A_2(r_{O_3} - A_3) + A_4(T - A_5) + A_6(\Sigma - A_7) + A_8r_{O_3}$$

 $A_1 = (P-L): \text{ Production and loss rate}$ $A_2 = \frac{\partial(P-L)}{\partial r_{O_3}}$ $A_3 = r_{O_3}: \text{ ozone mixing ratio}$ $A_4 = \frac{\partial(P-L)}{\partial T}$ $A_5 = T: \text{ temperature}$ $A_6 = \frac{\partial(P-L)}{\partial \Sigma}$ $A_7 = \Sigma: \text{ ozone column}$



Ai coefficients are monthly averages calculated with the MOBIDIC 2D model (Cariolle and Brard, 1984)

Cariolle, D. and H. Teyssèdre (2007). A revised linear ozone photochemistry parameterization for use in transport and general circulation models: multi-annual simulations. Atmos. Chem. Phys., 7, 2183–2196, 2007.





• Results and evaluation works



Results: Dust model

- Global and regional annual simulations evaluated with:
 - Aeronet sun-photometer networks
 - LIDAR vertical profiles



- Surface concentrations
- Emission and deposition fluxes







and do Supprogrammente

Pérez et al., 2011; Haustein et al., 2011





Aerosol optical depth near emission sources

Pérez et al., 2011 - ACPD

Results: Gas-phase chemistry

- Model setup:
- \rightarrow Global domain
- \rightarrow Non-hydrostatic physics
- → 1.4° x 1° horizontal resolution
- → 64 vertical (sigma-hybrid) layers
- → 1° x 1° NCEP/FNL analysis for meteorological initial conditions
- → Chemistry initial conditions from LMDz-INCA
- → Anthropogenic emissions: MOZART 2004
- → Biogenic emissions: MEGAN online model
- \rightarrow No biomass burning emissions
- → Half-year spin-up
- → July August 2004 simulation
- → All results are preliminary!



Preliminary evaluation with surface and ozonesondes



Evaluation against background surface from WDCGG, EMEP and CASTNET networks Evaluation from 3-hourly simulations

NO2			GAS (ppbv)	Source	N⁰ stns	Obs. Mean	Sim. Mean	MB	RMSE	MNBE (%)	MNGE (%)	MFB (%)	MFE (%)
			O3	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
со	Tabletis of solar to a finite solar part IN			CASTNET	63	31.73	33.86	2.37	2.21	11.57	22.67	7.58	20.56
			NO2	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
			СО	WDCGG	14	121.51	145.32	23.82	51.51	43.28	50.14	22.06	29.93

Root Mean Square Error(ppbv) in every station (<1000m) of Surface O3 (ppbv)



Root Mean Square Error(ppbv) in every station (<1000m) of Surface O3 (ppbv)

Root Mean Square Error(ppbv) in every station (<1000m) of Surface O3 (ppbv)-EMEP



Badia and Jorba, 2011 – EGU2011

Preliminary evaluation with surface and ozonesondes

Root Mean Square Error(ppbv) in every station (<1000m) of Surface O3 (ppbv)



Root Mean Square Error(ppbv) in every station (<1000m) of Surface O3 (ppbv)-EMEP





O3 (ppbv)





Box-and-whisker plot of vertical O3 (ppbv) profiles simulations over July-August 2004



Latitude (°)

Stratospheric ozone

- Implementation of the Cariolle and Teyssèdre (2007) linear model
- It improve the ozone balance within the troposphere









EP/TOMS Corrected Total Ozone Mar 1, 2004







• Future developments



Future developments (I/II)

- Improvement and evaluation of the chemistry part of the model.
- Implementation of the other global relevant aerosol species, i.e. sea-salt (SS), black (BC) and organic carbon (OC), and sulfate (SO4), in addition to dust (DU).
- It is planned to couple the radiative scheme with all the considered aerosol species to simulate the direct aerosol radiative effect.
- It is planned to couple the model ozone prediction with the radiative scheme of NMMB.
- It is panned to couple the photolysis scheme with the model clouds, ozone, and aerosol species (DU, SS, BC, OC, SO4).



Future developments (II/II)

- Implementation of secondary aerosol schemes (SIA, new SOA parameterizations) for LAM applications at high-resolutions
- Evaluation of the gas-phase chemistry on regional domains
- Experimental dust forecasts on global and regional domains to replace BSC-DREAM8b forecasts





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THANK YOU FOR YOUR ATTENTION

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Acknowledgments

This work was funded by grant CGL2006-11879, CGL2008/02818 and CGL2010/19652 of the Spanish Ministry of Science and Innovation.