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Memòria científica justificativa de la convocatòria de beques per a estades de recerca a l'estranger (BE-DGR)

La memòria justificativa consta de les dues parts que venen a continuació:
1.- Dades bàsiques i resums
2.- Memòria del treball (informe científic)

Tots els camps són obligatoris

1.- Dades bàsiques i resums

Títol del projecte: ha de sintetitzar la temàtica científica del vostre document.
Actualització del nucli meteorològic del model NMMB/BSC Chemical Transport Model

Dades de l'investigador o beneficiari

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Número d'expedient
2012BE100460

Paraules clau: cal que esmenteu cinc conceptes que defineixin el contingut de la vostra memòria.
Modelització numèrica; meteorologia; química atmosfèrica; models integrats; qualitat de l'aire

Data de presentació de la justificació
8/7/2013

Nom i cognoms i signatura de la
persona beneficiària de la beca

Generalitat de Catalunya
Departament d'Economia
i Coneixement

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Resum del projecte: cal adjuntar dos resums del document, l'un en anglès i l'altre en la llengua del document, on s'esmenti la durada de l'acció

Resum en la llengua del projecte (màxim 300 paraules)

El Departament de Ciències de la Terra del Barcelona Supercomputing Center desenvolupa el sistema de modelització NMMB/BSC Chemical Transport Model (NMMB/BSC-CTM). És un model de qualitat de l'aire multiescala i programat de forma integrada. El sistema de modelització representa una potent eina de reserca i permet realitzar modelitzacions a escala global i regional de la meteorologia, la qualitat de l'aire i la química atmosfèrica de forma eficient. Les escales de treball cobreixen des de escales sub-sinòptiques a mesoscalars. Les tasques realitzades durant la visita al centre NASA-GISS s'han centrat en l'actualització del model meteorològic emprat en el model NMMB/BSC-CTM. Aquest model meteorològic és el Nonhydrostatic Multiscale Meteorological model on the B grid (NMMB) desenvolupat pel National Centers for Environmental Prediction (NCEP). Durant la visita, la versió meteorològical del model NMMB/BSC-CTM s'ha migrat a la versió v2013 del model NMMB. Els mòduls de química gasosa, aerosols globals, aerosols secondaris s'han implementat de forma integrada (online) en la nova versió del model NMMB. El resultant model incorpora noves característiques d'execució com són la capacitat d'executar aniuaments des d'escales globals a locals, i incorpora una paral·lelització millorada. La visita s'ha realitzat entre el 3 de Març al 10 de Juny de 2013 al centre NASA Goddard institute for Space Studies (GISS) de Nova York.

Resum en anglès (màxim 300 paraules)

The Earth Sciences Department of the Barcelona Supercomputing Center develops the online multiscale air quality model NMMB/BSC Chemical Transport Model (NMMB/BSC-CTM). This new modelling system is intended to be a powerful tool for research and to provide efficient global and regional chemical weather simulations at sub-synoptic and mesoscale resolutions. The tasks undertaken during the visit to the NASA-GISS center were focused on the upgrade of the meteorological driver of NMMB/BSC-CTM. The meteorological driver is based on the Nonhydrostatic Multiscale Meteorological model on the B grid (NMMB) developed at National Centers for Environmental Prediction (NCEP). During the visit, the version v2013 of the NMMB has been implemented within the NMMB/BSC-CTM model. The gas-phase, global aerosols, secondary aerosols modules has been online integrated within the v2013 NMMB. The new version includes the capabilities of runing nests from global to local scales, and incorporates an improved paralelization of the modeling system. The visit took place from March 3rd to June 10th at the NASA Goddard Institute for Space Studies (GISS) of New York.

2.- Memòria del treball (informe científic sense limitació de paraules). Pot incloure altres fitxers de qualsevol mena, no més grans de 10 MB cadascun d'ells.

The main objective of the research visit is the upgrade of the meteorological version of NMMB/BSC-CTM model to the last release of the NMMB model (v2013) provided by NCEP. From this main objective the following specific objectives are identified:

- Review of the technical implementation of the gas-phase and aerosols within NMMB/BSC-CTM.
- Review of the technical structure of the new version of the meteorological model NMMB.
- Implementation of the gas-phase module in the new version of NMMB.
- Implementation of the aerosol module in the new version of NMMB.
- Development of the one-way and two-way interactions of the chemistry within NMMB/BSC-CTM upgraded system.
- Operational implementation of the new model version.

During the visit the main objectives has been achived. The meteorological driver of the model NMMB/BSC-CTM has been upgraded to the version v2013 of the NMMB model. Currently the nesting capabilities of NMMB are under development at NCEP, and only the one-way interaction approach has been implemented during this upgrade. The new modelling System NMMB/BSC-CTM provides operational forecasts of mineral dust for the Northern Africa-Middle East-Europe (NA-ME-E) Regional Center of the World Meteorological Organization (WMO). Model forecasts at both global and regional domains are available at http://www.bsc.es/earth-sciences/mineral-dust/nmmbbsc-dust-forecast/.

Task 1. Analysis of the structure of the models

The structure of the NMMB/BSC-CTM model and the new version of the NMMB model have been reviewed to design the approach of the upgrade. Regular contacts with NCEP modelers have been mantained during the visit.

Figure 1 shows the structure of the previous NMMB model (v2009) and the integration of the aerosols and chemistry. These were the initial structures of the modelling systems at the start of the visit. The initial version of NMMB/BSC-CTM was structured in two main modules: (1) Dynamics, (2) Physics. In the Dynamics module all the routines involved in the solution of the adiabatic primitive equations are included. Indeed, the horizontal diffusion, horizontal advection, vertical advection, and tracer monotonization are the processes solved in Dynamics and related with the transport of the chemical tracers. On the other hand, the Physics module contains all the diabatic terms of the primitive equations. In this sense, the radiation, turbulence (surface layer, planetary boundary layer, land surface model), convection, and microphysics processes are included. The global aerosols dry and wet deposition, emissions, and sedimentation processes are included in the Physics module. All the gas-phase and secondary-aerosols chemistry are implemented at the end of Physics module.

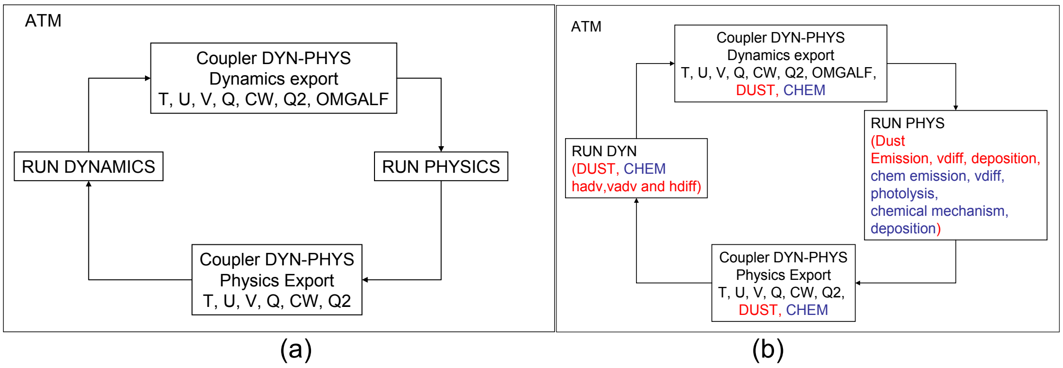

Figure 1. (a) Structure of the NMMB v2009 model, (b) structure of the NMMB/BSC-CTM model.

Figure 2 shows the sequence call of subroutines of the NMMB/BSC-CTM model. The Dynamics part is executed in a first place followed by the Physics part. At the end the gas-phase chemistry routines are executed. The green color indicates those subroutines associated with a process involving the gas or aerosol chemistry.

	DYN in UMO	
only first step	PGFORCE	Pressure gradient routine
	DHT	Divergence and horizontal pressure advection in thermo equation
if not first step	HDIFF	Horizontal diffusion
	READ_BC	Read boundary conditions for regional forecast and update the mass points
	BOCOH	Updating boundary values at height points
	PGFORCE	Pressure gradient routine
	UPDATEUV	Update the wind field
	BOCOV	Update the boundary velocity points for the regional forecast
	DHT	Divergence and horizontal advection in thermo equation
	DDAMP	Divergence damping
all steps	PDTSDT	Update the surface pressure
	ADV1	Advection of T, U and V
	ADV2	Advection of tracers
	MONO	Tracer monotonization
	UPDATES	Updates tracers Q, CW, RRW, Q2
	VTOA	Interface pressures and horizontal part of omega-alpha term
	UPDATET	Update temperature field
	CDZDT	Nonhydrostatic advection of height
	CDWDT	Advection of W
	VSOUND	Vertically propagating fast waves
	VADV2	Old vertical advection of passive quantities
	HADV2	Old horizontal advection of passive quantities
	PHYS in UMO	
	RADIATION	Radiation
	RDTEMP	Update the temperature with the radiative tendency
	TURBL	Turbulence, SFC layer, and land surface - vertical diffusion
	CUCNVC	Convection
	GSMDRIVE	Microphysics
	CHEM in UMO-CHEM	
Chem module	EMI	Emission driver
	PHOT	Photolysis scheme
	DRYDEP	Dry deposition
	CNVTRP	Convective transport
	WETDEP	Wet deposition
	CHEM	Chemical mechanism

Figure 2. Sequence of subroutine calls of the NMMB/BSC-CTM v2009.

The new version of the NMMB v2013 has substantially been restructured. Now the meteorological model contains only one main module named Solver. The new Solver module includes both Dynamics and Physics previous modules. This new structure simplifies the definition of variables and exchange of information between the dynamics and physics routines. Additionally, several model drivers have been substantially simplified. Each physics subroutine has a driver where all the required variables are prepared. The new version simplifies this step, and a direct coupling is now implemented. Another important change identified with v2013 is the implementation of the nesting capabilities. The model has the one-way, moving nest, and two-way nesting options. Currently, the two-way option is under development.

In the NMMB v2013 the model exploites the Earth System Modeling Framework (ESMF) capabilities in more depth. The ESMF structure allows to execute the model in ensemble configuration (several runs at once), the coupling with an ocean model, and the execution of nesting domains. The nesting driver routines are implemented within the Solver module.

Task 2. Design of the modelling system upgrade

The design of the upgrade follows the same philosophy of NMMB/BSC-CTM. The gas and aerosol modlues are programed within the code of the meteorological driver. The global aerosol processes will be inlined within the meteorological subroutines, in this sense, the emissions, dry deposition, wet deposition, and radiative interactions are inlined in TURBL, CUCNVC, GSMDRIVE and RADIATION respectively. The gas-phase chemistry subroutines are included after the call sequence of physics.

Figure 3 shows the new sequence of subroutine calls in the new version of the model NMMB/BSC-CTM v2013. Now all the relevant subroutines are included in the module SOLVER. The green color indicates those processes where the chemistry gas and aerosol tracers are involved. Compared with Figure 2, some specific subroutines associated with nesting tasks are now included (READ/WRITE_BC_CHEM, BOCOH_CHEM). Also, the initialization and spin-up of the chemistry is called at the beginning of the SOLVER module (COUPLE_SPINUP_DUST, CHEMISTRY_INITIALIZE). The advection of chemistry tracers are now implemented in a separated subroutines (ADV2_CHEM, MONO_CHEM, UPDATES_CHEM). All the global aerosol processes are inlined within the meteorological subroutines. A new SEDIMENTATION subroutine is called after RADIATION. Following the same approach as the initial version, the CHEM_DRIVER subroutine is called at the end of the physics subroutines.

	SOLVER in UMO	
only first step	PGFORCE	Pressure gradient routine
	DHT	Divergence and horizontal pressure advection in thermo equation
if not first step	COUPLE_SPINUP_DUST	Spin up of global aerosols
	CCHEMISTRY_INITIALIZE	Initialization of chemistry arrays
	HDIFF	Horizontal diffusion
	READ_BC/WRITE_BC	Read/write boundary conditions and update the mass points
	READ/WRITE_BC_CHEM	Read/write boundary conditions of chemical species
	BOCOH	Updating boundary values at height points
	BOCOH_CHEM	Updating boundary values of chemical species
	PGFORCE	Pressure gradient routine
	UPDATEUV	Update the wind field
	BOCOV	Update the boundary velocity points for the regional forecast
	DHT	Divergence and horizontal advection in thermo equation
	DDAMP	Divergence damping
all steps	PDTSDT	Update the surface pressure
	ADV1	Advection of T, U and V
	ADV2	Advection of tracers
	MONO	Tracer monotonization
	UPDATES	Updates tracers Q, CW, RRW, Q2
	ADV2_CHEM	Advection of tracers
	MONO_CHEM	Tracer monotonization
	UPDATES_CHEM	Updates tracers Q, CW, RRW, Q2
	VTOA	Interface pressures and horizontal part of omega-alpha term
	UPDATET	Update temperature field
	CDZDT	Nonhydrostatic advection of height
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	VSOUND	Vertically propagating fast waves
	RADIATION	Radiation
	RDTEMP	Update the temperature with the radiative tendency
	SEDIMENTATION	Sedimentation of aerosols
	TURBL	Turbulence, SFC layer, and land surface - vertical diffusion
	CUCNVC	Convection
	GSMDRIVE	Microphysics
	CHEM_DRIVER	
	EMI	Emission driver
	PHOT	Photolysis scheme
	DRYDEP	Dry deposition
	CNVTRP	Convective transport
	WETDEP	Wet deposition
	CHEM	Chemical mechanism
	AERO_CHEM	Secondary aerosol mechanism

Figure 3. Sequence of subroutines calls of the new version of the NMMB/BSC-CTM model with NMMB v2013.

The implementation of the aerosol and gas chemistry subroutines have been done following the order: (1) coupling the gas-phase chemistry, (2) coupling the global aerosol module.

Task 3. Porting the gas-phase chemistry module to the new NMMB model

The gas-phase processes are programed in a modular approach. There is a principal driver, CHEM_DRIVER, that contains all the subroutine calls of the gas-phase chemistry processes and the secondary aerosol mechanism: (1) EMISSIONS, (2) DRY DEPOSITION, (3) WET DEPOSITION, (4) GAS PHASE CHEMICAL MECHANISM, (5) SECONDARY AEROSOL CHEMICAL MECHANISM. The implementation of the main subroutines has been straightforward. Most of the efforts has been spent in the reprograming of the initialization of the chemistry and the spin-up and nesting capabilities.

Concerning the nesting capabilities, the work was started during the visit and is under development nowadays. The nesting structure is quite complex and the inclusion of chemical tracers requires important efforts of programming and debugging.

Figure 4 shows some results of the photolysis rates of NO_2 computed with the new implementation. Such results are nearly identical from the previous version of the model. It is important to note that the new version allows the application of a more complex radiative parametrization, the RRTMG. This new parametrization allows the interaction of aerosols with radiation.

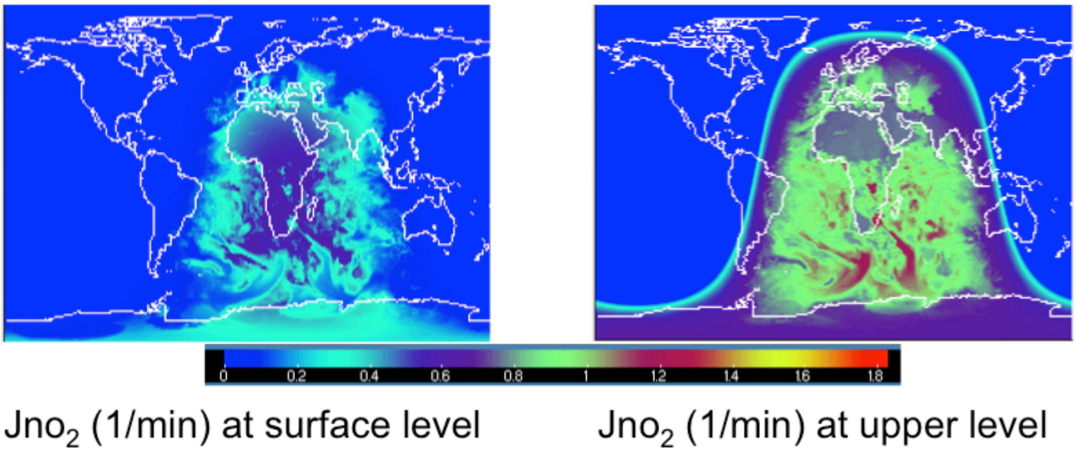


Figure 4. NO_2 photolysis rate at surface level (left) and at the top of the model (right).

Task 4. Porting the global aerosol module to the new NMMB model

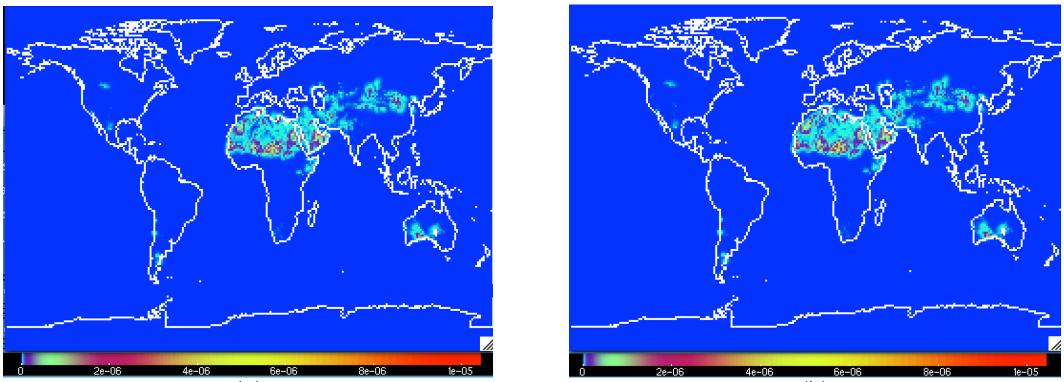
The global aerosol module of the system currently includes the processes of emission, transport and deposition of mineral dust aerosol and sea-salt aerosol. The initial work was dedicated to implement all the processes associated with the mineral dust. Thus, the emission scheme was implemented within the turbulence subroutine. Such emission scheme is directly coupled with the surface viscous sublayer of the meteorological driver. After that, the dry deposition and sedimentation subroutines were coded just after the turbulence. The wet deposition processes were inlined within the convective subroutine and the microphysics subroutine. Thus, the convective mixing, incloud and below cloud scavenging for both grid and sub-grid scale clouds were implemented.

Figure 5 shows the results of a 12h simulation of mineral dust using v2009 and the new model version v2013. The main structures are maintained. Small differences are attributed to the new meteorology. Overall, the porting of the mineral dust shows good results and reproduce previous results of the model.

During the porting of the mineral dust, some minor errors where detected in the v2009. Those were corrected then in v2013. An example is the treatment of the transport of the passive tracers within NMMB. The equations of the model considers the tracer represented as a mixing ratio [kg tracer/kg air]. V2009 was using aerosol concentration [kg m-3] instead of mixing ratio. This may have some impact in upper layers of the model, where the air density is significatively minor of 1.

Following the implementation of the mineral dust module, the sea-salt aerosol was implemented in the new model version. Main differences with the mineral dust aerosol are the emission scheme, and the hygroscopic growth of the sea-salt aerosol. The latter affects the sedimentation, convective mixing, incloud and below cloud scavenging. Following the philosophy of the mineral dust implementation, the sea-salt processes are also inlined within the meteorology subroutines.

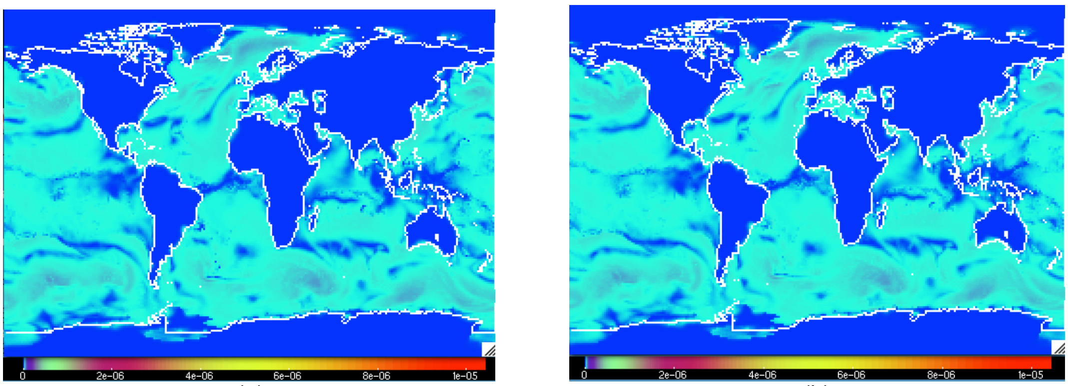
A drawback of the sea-salt implementation in model v2009 was the way some processes were programmed. A hardwired approach was used with the sea-salt, and there was no option to run the module turning off the dust aerosol if the user were interested on it. In the new version, v2013, this has been corrected. Now, the model can be configured turning on or off any of the aerosols implemented. And has been prepared for the future implementation of Black carbron, Organic carbon, and Sulphate aerosols.



(a) (b)

Figure 5. Mineral dust aerosol concentration [kg m-3] of bin number 5 (1 to 1.80 μm) at surface layer for (a) model version 2009, and (b) new model version v2013.

In Figure 6 results from v2009 and v2013 are shown. The sea-salt concentration of bin number 5 at surface layer are depicted for both model versions at 12h of a model simulation. Again, the differences between the two model versions are minor and attributed to the new meteorology. Several tests have been performed to check the correctness of the implementation in the v2013 version.



(a) (b)

Figure 6. Sea-salt aerosol concentration [kg m-3] of bin number 5 (1 to 1.80 μm) at surface layer for (a) model version 2009, and (b) new model version v2013.

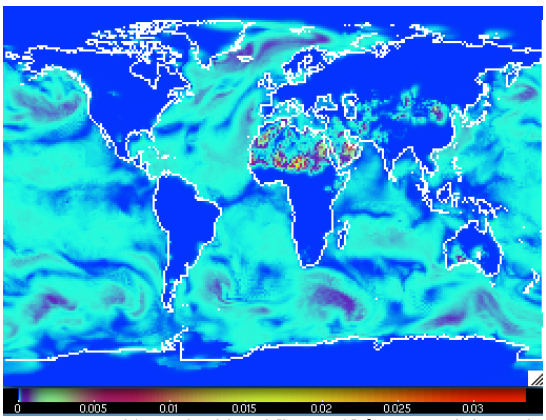


Figure 7. Aerosol (mineral dust + sea-salt) vertical load [kg m-2] from model version 2013.

Finally, Figure 7 shows the results of a simulation with v2013 model version, where both the mineral dust and the sea-salt aerosols are turned on. The Figure presents the aerosol vertical load [kg m-2] for a 12h simulation. Results are in agreement with the model results of v2009. Higher aerosol loads are identified over Northern Africa and Arabian Peninsula. The aerosol load of the sea-salt aerosol is lower than the mineral dust in source regions.

Task 5. Testing of the upgraded model: global, regional, and nesting capabilities for the chemistry species

The NMMB/BSC-CTM v2013 has been initially tested during the last weeks of the visit. The global configuration, regional configuration were tested. The nesting capabilities for the aerosol and gases are currently under development and under debugging. Runs activating the gas-phase chemistry were performed for a global domain configuration and an European domain configuration. In the same way, runs turning on the mineral dust aerosol were performed.

Here we show some results of the model for the global configuration and regional configuration for chemistry gases (ozone and NO_2), mineral dust, and sea-salt aerosols. Again, results are in agreement with previous runs performed with v2009 model. From those runs, the model v2013 is 20% faster than with v2009. This is attributed to the simplification of the model structure and the limitation of the all-to-all mpi communications. Additionally, the suppression of some parameterization drivers contributes to that speed-up.

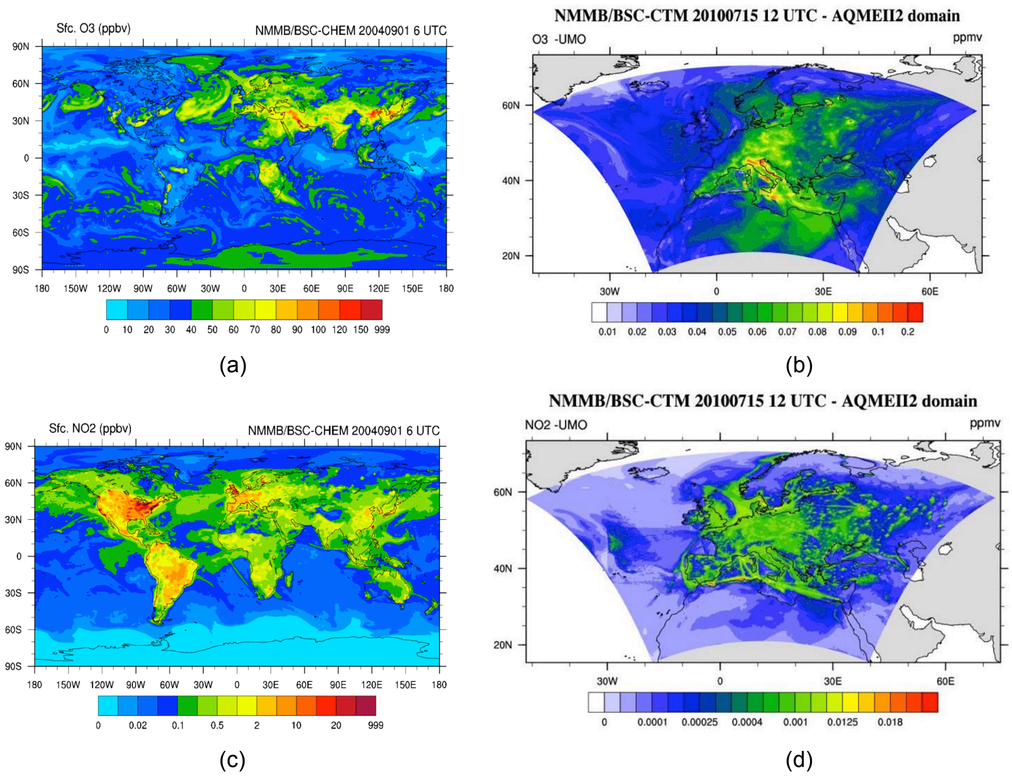


Figure 8. Results of NMMB/BSC-CTM v2013 configured with the gas-phase chemistry turned on for a global and a regional domain. (a) and (c) show ozone surface concentration and NO2 surface concentration for a global domain at coarse resolution (1ºx1.4º). (b) and (d) show ozone and NO2 surface concentration for an European domain at high resolution (12 km).

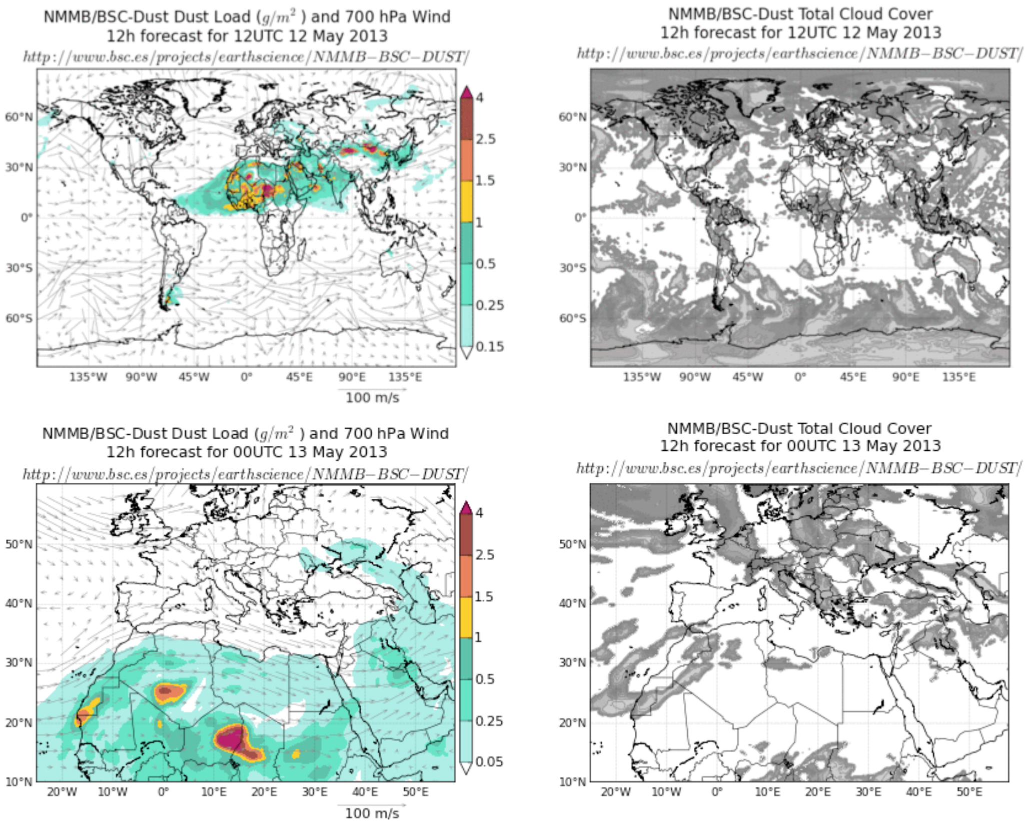


Figure 9. Global (upper panels) and regional European domain (below panels) results of mineral dust vertical loads with the v2013 NMMB/BSC-CTM model version. The figures uses the same design as the ones provided in the web page of the Earth Sciences Department forecasts.

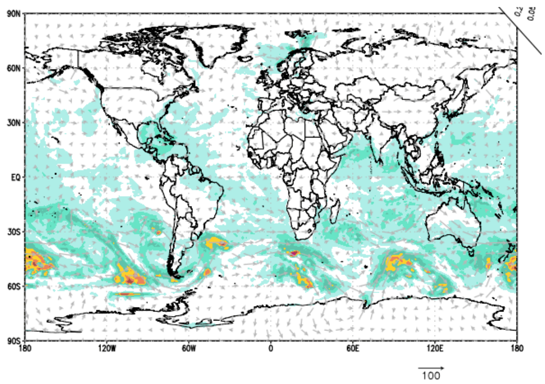


Figure 10. Global simulation of sea-salt vertical load with the v2013 NMMB/BSC-CTM model version.

Task 6. Implementation of the upgrade version of NMMB/BSC-CTM as experimental forecasting system for aerosol predictions

The implementation of the new version of the model will be implemented in the forecasting system of the Earth Sciences Department of the Barcelona Supercomputing Center. Although we initially include this task to be started during the visit, the work was focused in the model development and no time left was available to start the task. During July-September the model will be implemented in forecast mode and extensively evaluated.

The new model NMMB/BSC-CTM will contribute to the international initiatives of model intercomparison and model forecasts undertaken by the Earth Sciences Department of the BSC:

- Mineral dust aerosol forecasts for the WMO *Sand and Dust Storm Warning Advisory and Assessment System* (SDS-WAS) - *Northern Africa-Middle East-Europe (NA-ME-E) Regional Center*.
- Base model of the recently created WMO *Regional Specialized Meteorological Centre for Specialized Activity on Atmospheric Sand and Dust storm Forecasts of Barcelona*.
- Participation on the AQMEII-Phase2 online chemical transport model intercomparison initiative.
- Participation on the ICAP global aerosol model intercomparison initiative.