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Update on the developments of aerosol and gas chemistry processes inlined within the NMMB multiscale model at the Barcelona Supercomputing Center

O. Jorba

Earth Sciences Department
Barcelona Supercomputing Center

Acknowledgments: Z. Janjic, C. Pérez, S. Basart, A. Badia, M. Spada, J.M. Baldasano, D. Dabdub, K. Haustein, T. Black, E. Tarradellas, F. Benicasa

Outline

- « BSC and the Earth Sciences Department
- « The NMMB/BSC-Chemical Transport Model
 - Mineral Dust Results
 - Sea Salt Aerosol results
 - Gas-phase results
- « Future work



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BSC AND THE EARTH SCIENCES DEPARTMENT

BSC-CNS

- Barcelona Supercomputing Center – Centro Nacional de Supercomputación (BSC-CNS) is the Spanish National Laboratory in supercomputing.

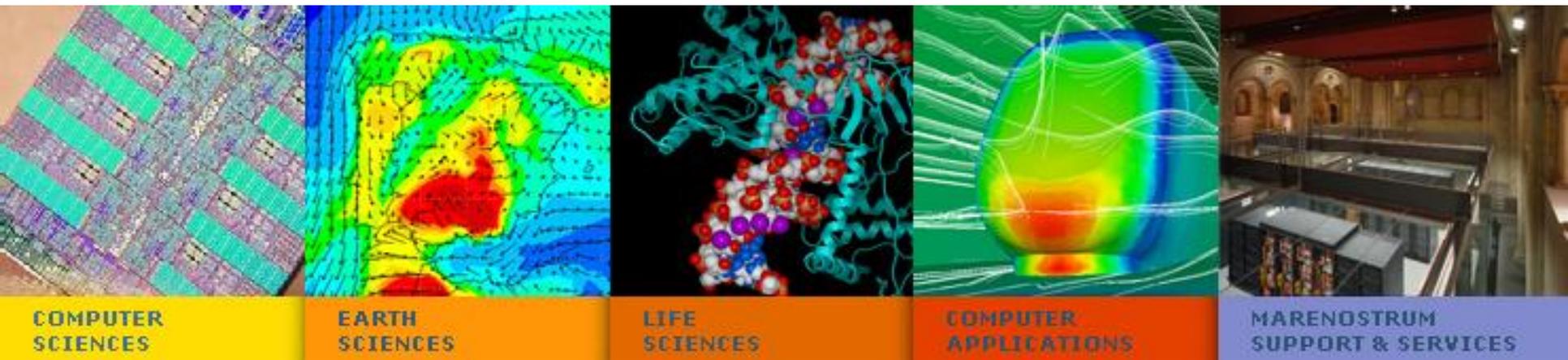


- The BSC mission:
 - To investigate, develop and manage technology to facilitate the advancement of science.
- The BSC objectives:
 - To perform R&D in Computer Sciences and e-Sciences
 - To provide Supercomputing support to external research.
- BSC is a consortium that includes:
 - the Spanish Government – 51%
 - the Catalan Government – 37%
 - the Technical University of Catalonia – 12%



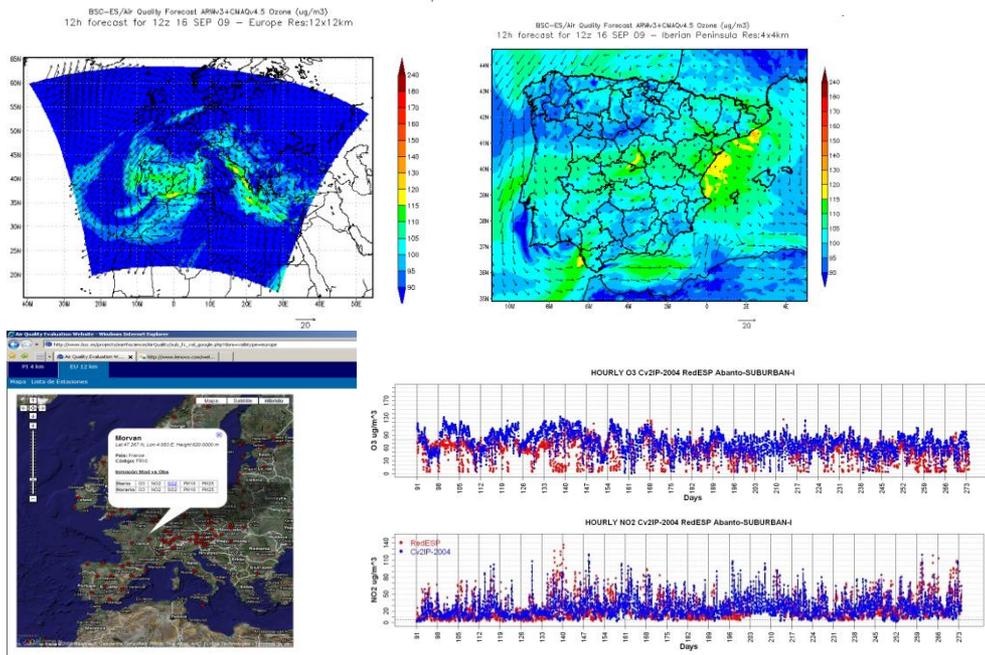
BSC Scientific & Technical Departments

The BSC is a fusion of a classic Scientific Support Structure and a classic Research Institute.



www.bsc.es

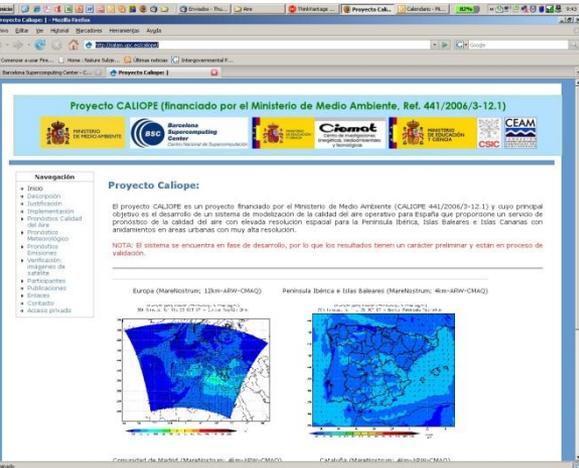
Research in the Earth Sciences area is devoted to the development and implementation of regional and global state-of-the-art models for short-term air quality forecast and long-term climate applications.



ES maintains two daily operational systems: AQF CALIOPE and MD forecasts: BSC-DREAM8b and NMMB/BSC-CTM.

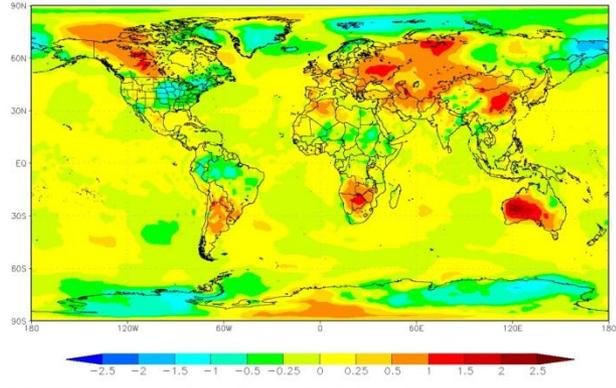
Earth Sciences research lines

Air Quality Forecast



Climate change modelling

GISS ModelE at BSC-CNS Surface Temperature Anomaly C (1951-1980)
Year 1956, BAU scenario - Global Res:2x2.5

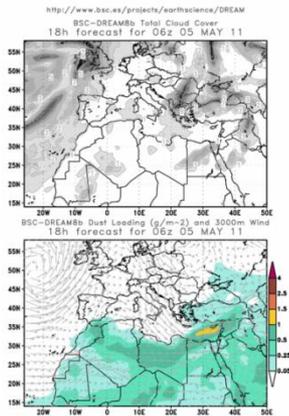


Transfer technology (EIA and AQ studies)

EIA- Modelización Calidad del Aire
Localización de los EIA



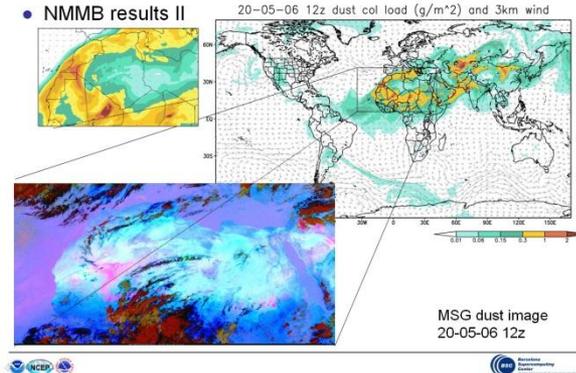
Mineral dust transport: BSC-DREAM8b



Atmospheric modelling: development of NMMB/BSC-CTM

NMMB/BSC-DUST

NMMB results II



WMO SDS WAS [AEMET-BSC]

WMO Sand and Dust Storm Warning and Assessment System (SDS WAS)

- To enhance the ability of participating countries to establish and improve systems for forecasting and warning to suppress the impact of Sand and Dust Storm by
- Establishing a coordinated global network of Sand and Dust Storm forecasting centers delivering products useful to a wide range of users in understanding and reducing the impacts of SDS





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NMMB/BSC CHEMICAL TRANSPORT MODEL

NMMB/BSC project

- ❧ Memorandum of understanding NCEP – BSC on the use and development of air quality and meteorological modules within the new NMMB NWP model (2009-2013)

- ❧ 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 atmospheric global-regional umo/dream model [CICYT CGL2008-02818].
 - Coupling of a fully online multi-component aerosol module within the atmospheric global-regional NMMB model [CICYT CGL2010-19652].
 - Severo-Ochoa Centre of Excellence

- ❧ Development under a collaborative framework with several research institutions

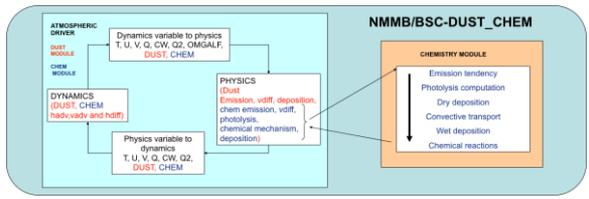
- ❧ Experimental research regional and global air quality modelling system

NMMB/BSC-Chemical Transport Model (Overview)

- fully on-line access coupling: feedback processes allowed
- multiscale: global to regional scales allowed

→ Janjic and Gall (NCAR/TN 2012)
 → Janjic and Vasic (EGU2012)
 → Janjic et al. (MWR 2011)
 → (...)

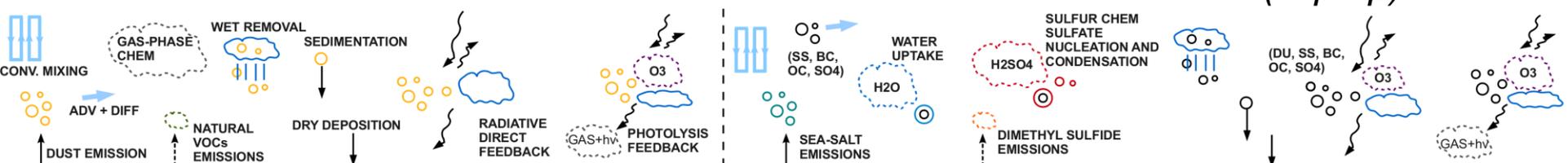
Nonhydrostatic Multiscale Model on the B-grid (NMMB) meteo variables/parameters



NMMB/ BSC-CTM

BSC Chemical Transport Model (gas/aerosol variables: mass mixing ratios)

- GAS-PHASE CHEM** (52 species) → Jorba et al. (JGR 2012)
- DUST** (8 bins) → Pérez et al. (ACP 2011)
 → Haustein et al. (ACP 2012)
- SEA-SALT** (in prep) → Spada et al.



NMMB/BSC-Chemical Transport Model

⌘ Mineral Dust module – NMMB/BSC-Dust (Pérez et al., 2011; Haustein et al., 2012)

- Evolution of the BSC-DREAM8b model (Nickovic et al., 2001; Pérez et al., 2006)
- Implementation of all common on-line dust modules for global and regional simulations
- Current DREAM dust emission scheme upgraded to a physically based scheme (explicitly accounting for saltation and sandblasting)
- New high resolution database for soil textures and vegetation fraction
- Direct radiative effect implemented

⌘ Gas phase chemistry (Jorba et al., 2012)

- Integrated implementation within NMMB – chemistry solved after NMMB physics
- Consistent advection and diffusion schemes with meteorology
- Feedback interactions aerosols-photolysis allowed
- Processes implemented online: emission, chemistry, dry and wet deposition each time-step. Online biogenic emissions from MEGAN

⌘ Global relevant aerosol module (Spada et al., 2013)

- Complementing NMMB/BSC-DUST mineral dust aerosols
- Same numerics like dust implementation
- Inclusion of Sea Salt, BC, OC and sulfate
- Implementation of feedbacks foreseen

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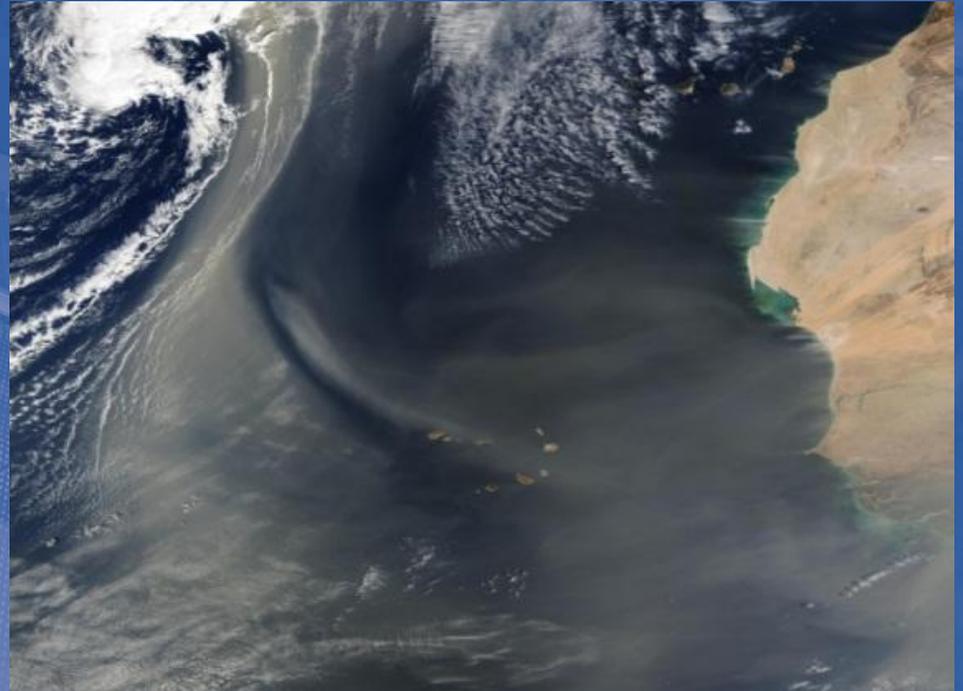
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MINERAL DUST MODULE

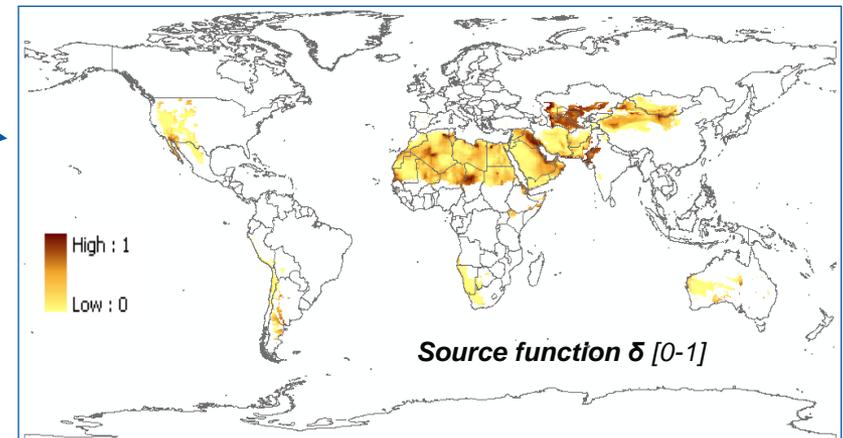
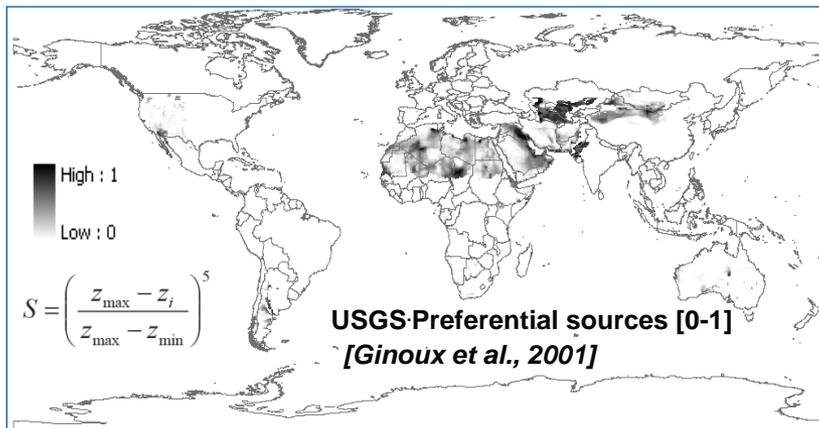
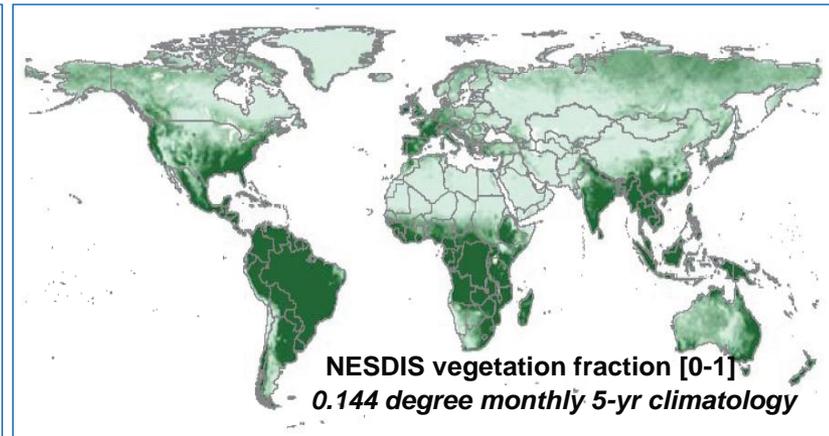
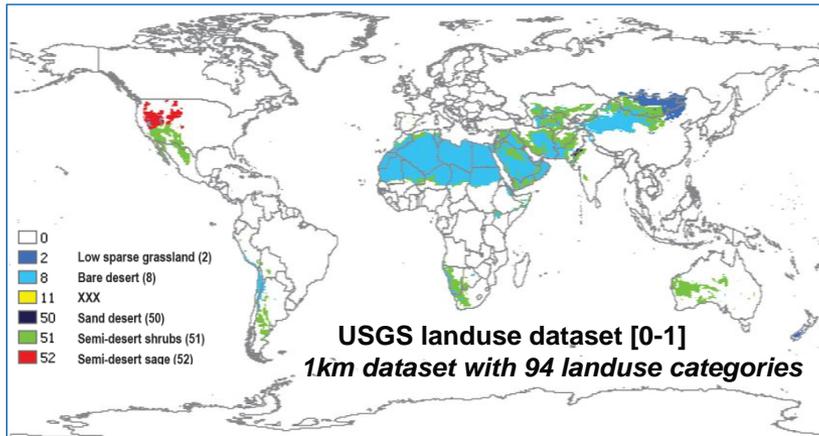
The NMMB/BSC-DUST model

NMMB/BSC-DUST is embedded into the NMMB model and solves the mass balance equation for dust taking into account the following processes:

- Dust generation/emission by surface wind
- Horizontal and vertical advection
- Vertical transport/diffusion by turbulence and convection
- Dry deposition and gravitational settling
- Wet removal including in-cloud and below-cloud scavenging
- RRTM SW/LW dust radiative feedback

The NMMB/BSC-DUST model: Emission scheme

Source function: update databases



$$\delta = USGS \cdot PREF \cdot (1 - VEGFRAC) \cdot (1 - SnowCover)$$

The NMMB/BSC-DUST model: Emission scheme

Dust generation/emission by surface wind

- Threshold friction velocity (Iversen and White, 1982; Marticorena and Bergametti, 1995)

$$u_{*total}(D, z_0, w) = \frac{u_{*dry}^{MB}(D)}{R(z_0, z_{0S})} \cdot H(w)$$

H=Moisture correction
R=Drag partition correction

- Horizontal flux (White, 1979)

$$H = \frac{\rho_{air}}{g} \cdot u_*^3 \cdot \sum_i \left(\left(1 + \frac{u_{*total}}{u_*} \right) \cdot \left(1 - \frac{u_{*total}^2}{u_*^2} \right) \cdot s_i \right)$$

H=Horizontal dust flux
s_i=relative surface area of each parent soil fraction

- Vertical flux (Shao et al., 1993; Marticorena and Bergametti, 1995, Tegen et al., 2002)

$$F_s = C \cdot \alpha \cdot \delta \cdot H$$

F_s=Vertical surface dust flux;
α=horizontal to vertical flux ratio;
δ=Source function

- Viscous sublayer effects near the surface (Janjic, 2001)

The NMMB/BSC-DUST model: Deposition scheme

- Dry deposition and gravitational settling

- Gravitational settling or sedimentation (Slinn, 1982)

$$v_{gk} = \frac{d_k^2 g (\rho_k - \rho_a) C_c}{18\nu} \quad C_c = \text{Cunningham correction}$$

- Dry deposition (Zhang et al., 2001): Brownian diffusion, interception and impaction are considered.

$$v_{dk} = v_{gk} + \frac{1}{(R_a + R_s)}$$

- Wet removal including in-cloud and below-cloud scavenging

- Dust scavenging is computed separately for convective and grid-scale precipitation
- Ferrier grid-scale microphysics and Betts-Miller-Janjic convective adjustment scheme
- Below cloud scavenging in each layer (Slinn, 1984; Loosmoore and Cederwall, 2004)

The NMMB/BSC-DUST: Model configuration

Global configuration:

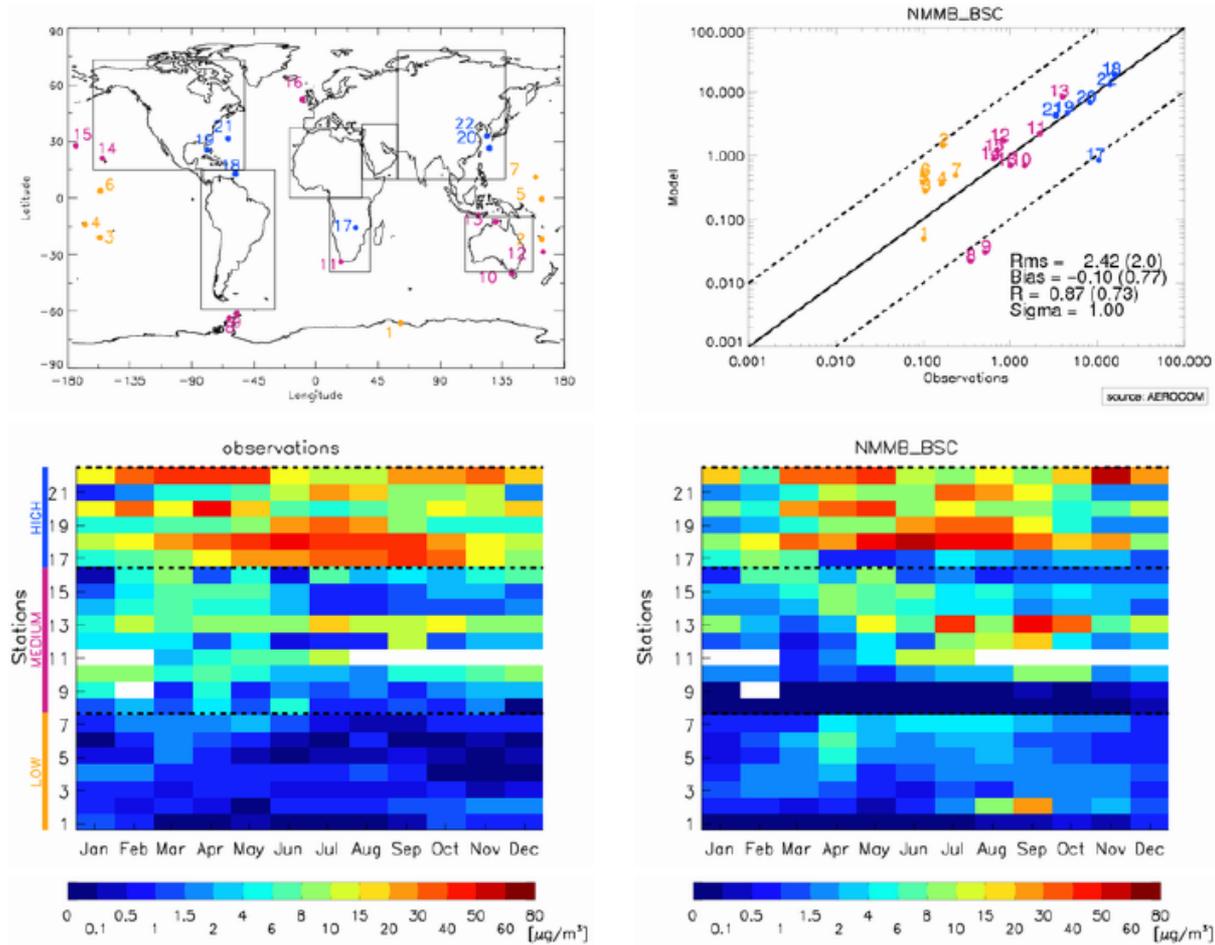
- Global domain at $1.4^\circ \times 1^\circ$ horizontal resolution
- 24 vertical levels
- fundamental time step of 180s
- Cold start without data assimilation
- Initial conditions from NCEP meteorological analysis $1 \times 1^\circ$ and Meteorological fields updated with NCEP every 24 h
 - *Annual simulation: 2000*

Regional configuration:

- North African domain at $0.25^\circ \times 0.25^\circ$ horizontal spatial resolution
- 40 vertical layers
- fundamental time step of 40s
- Cold start without data assimilation
- Initial conditions from NCEP meteorological analysis $1 \times 1^\circ$ and meteorology fields updated boundary conditions every 6 h
 - *Annual simulation: 2006*
 - *SAMUM-I period May 2006*
 - *BoDEx period March 2005*
 - *Dust storm in March 2004*

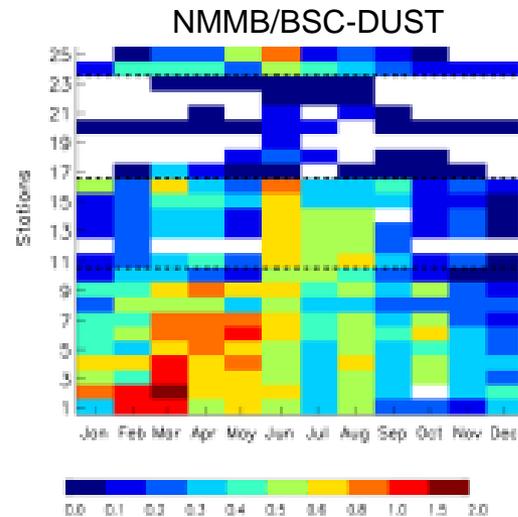
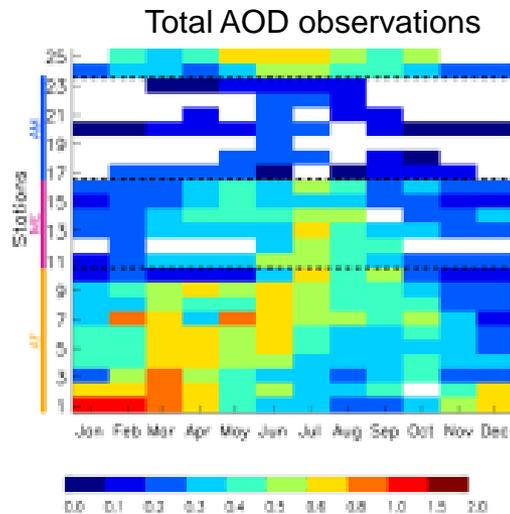
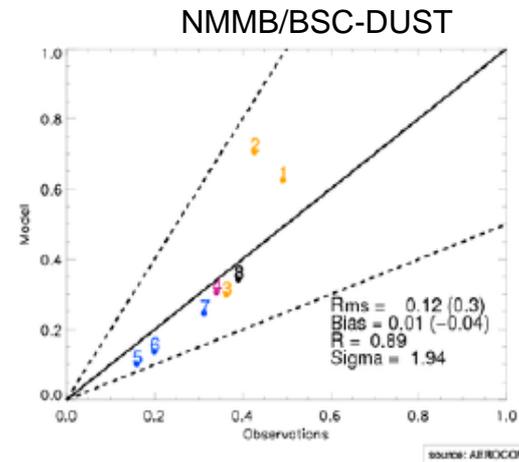
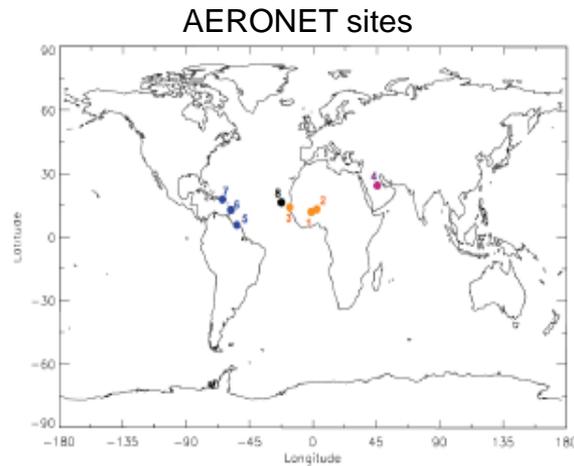
The NMMB/BSC-DUST: Global domain

Surface concentration for 2000 (Pérez et al., 2011)



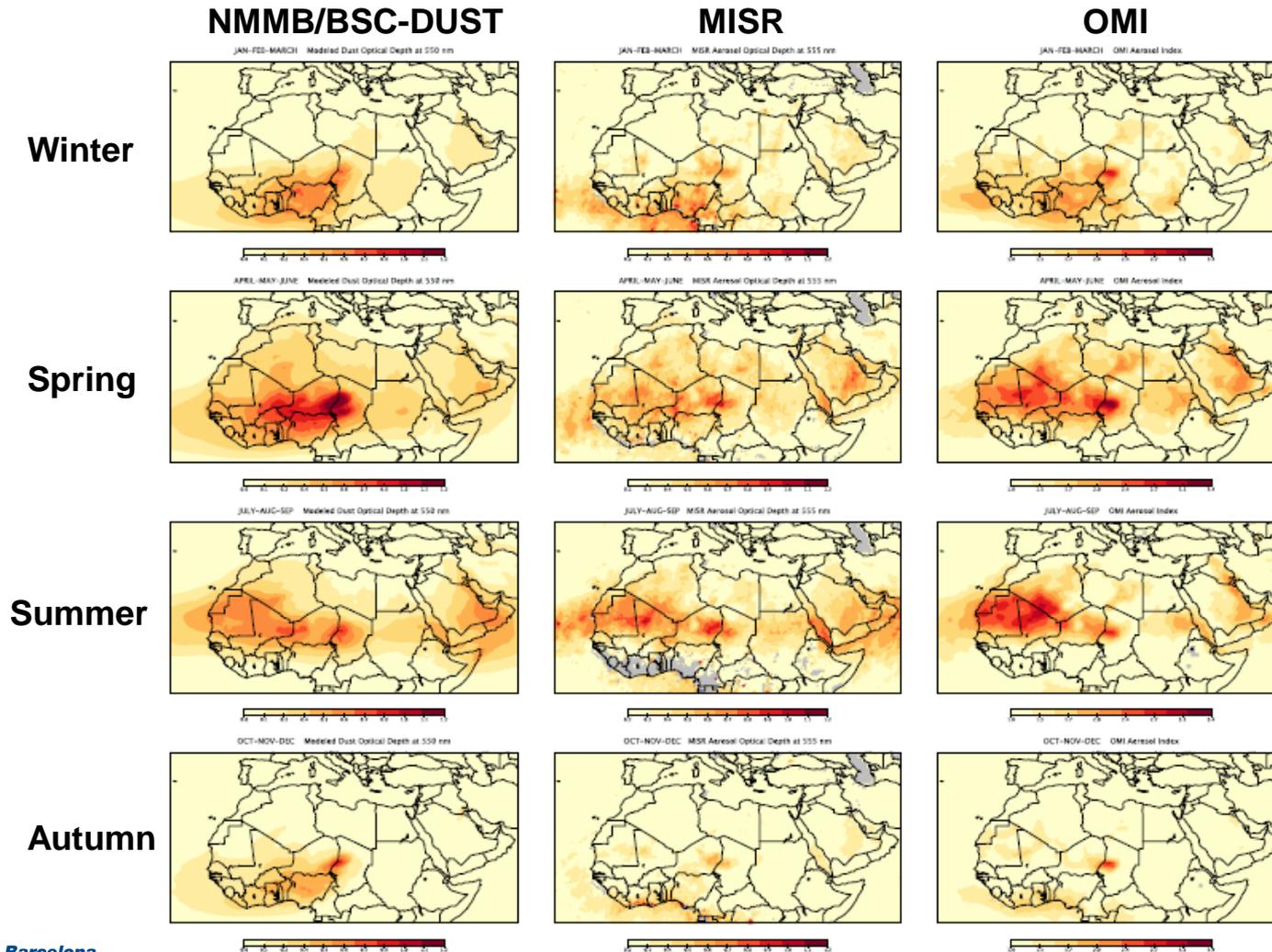
The NMMB/BSC-DUST: Global domain

AOD for 2000 vs. Climatology 1996-2006 (Pérez et al., 2011)



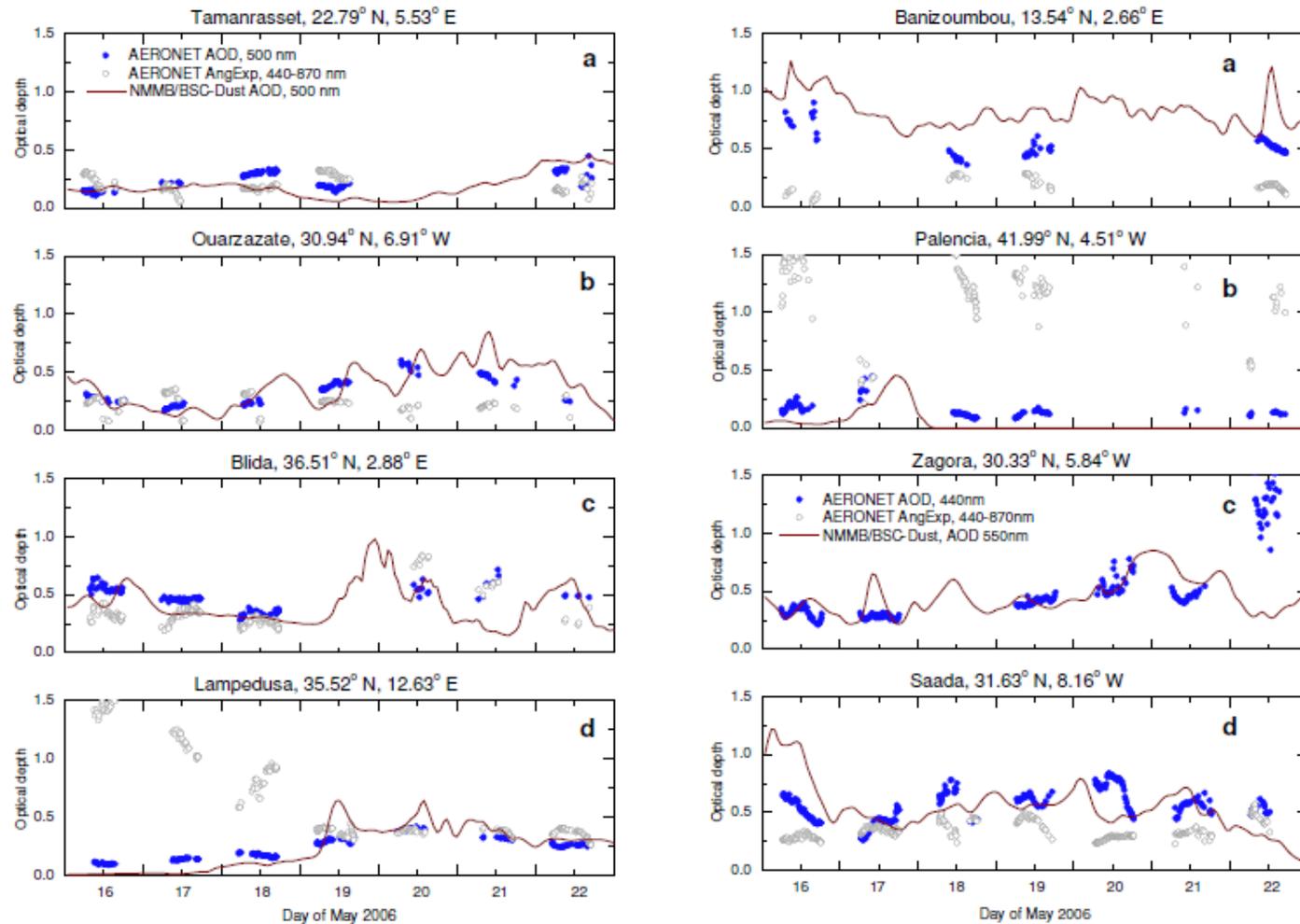
The NMMB/BSC-DUST: Regional domain

Satellite comparison for 2006 (Pérez et al., 2011)



The NMMB/BSC-DUST: Regional domain

SAMUM-I May 2006 – AERONET (Haustein et al., 2012)





World Meteorological Organization
Member of UNESCO - WHO

NORTHERN AFRICA-MIDDLE EAST-EUROPE (NA-ME-E) REGIONAL CENTER

WMO Sand and Dust Storm Warning Advisory and Assessment System (SDS-WAS)

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WMO SDS WAS | Asia Regional Center





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Feb 25, 2013

[UNEP Global Environmental Alert Service releases 'Forecasting and early warning of dust storms'](#)
Feb 18, 2013

[Scholarship on desert dust at the Univ. of Reading, UK](#)

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DUST FORECASTS

DUST OBSERVATIONS

GUIDANCE FOR FORECASTERS

TIME-AVERAGED VALUES

FORECAST EVALUATION

REANALYSIS

DATA POLICY

Multimodel Products

WMO SDS-WAS NA-ME-E Regional Center will be a Regional Specialized Meteorological Center

Forecast evaluation

Compared dust forecasts

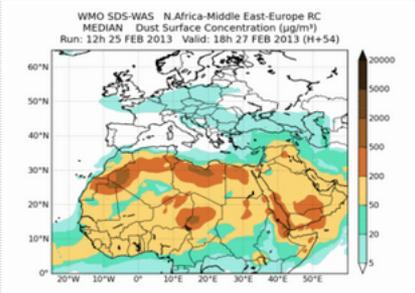
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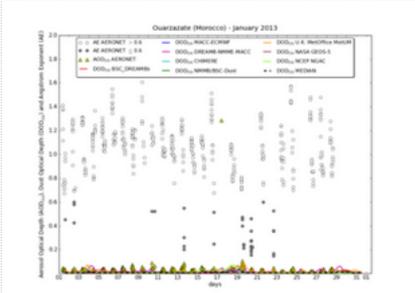
To be informed about our activities, news and events related to dust. Frequency is almost monthly.

Full Name

Your email

Dust forecasts





SDS-WAS RC: DUST MODELS



LMD



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LSCE



mac
Monitoring atmospheric
composition & climate



Met Office



SEEVCCC



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NCEP

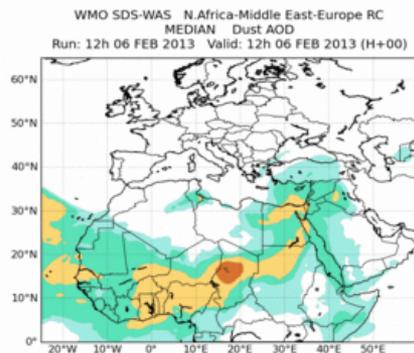
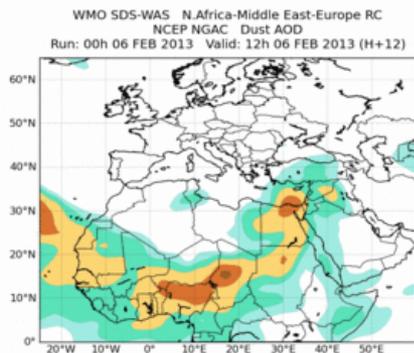
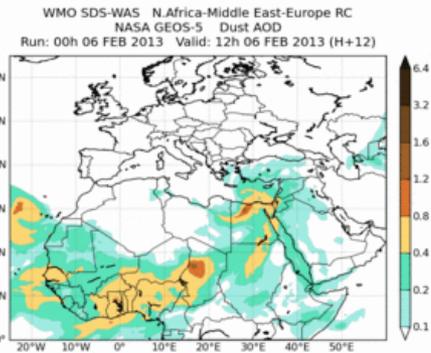
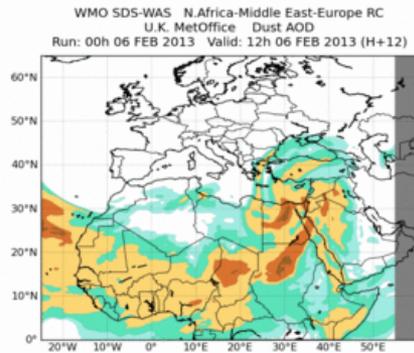
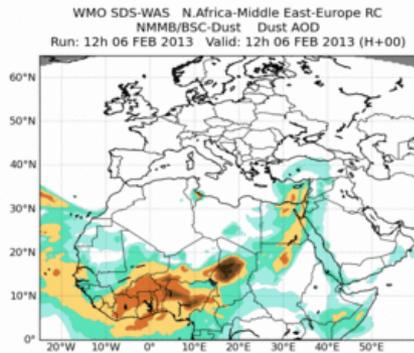
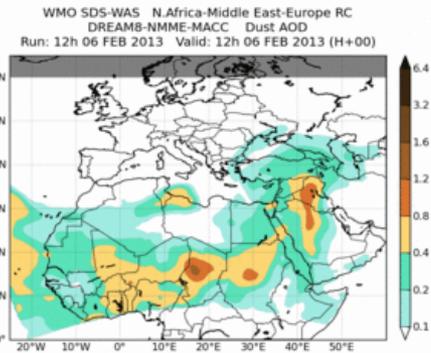
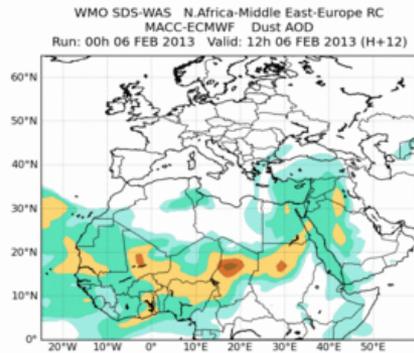
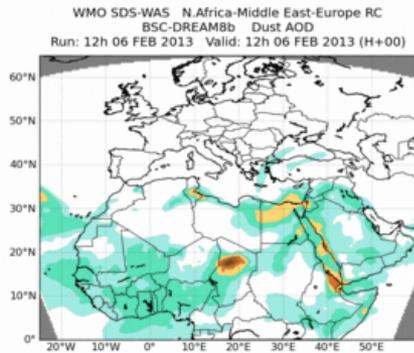
MODEL	INSTITUTION	RUN TIME	DOMAIN
BSC-DREAM8b	BSC-CNS	12	Regional
NMMB/BSC-Dust	BSC-CNS	12	Regional
DREAM-NMME-MACC	SEEVCCC	12	Regional
CHIMERE	LMD	00	Regional
LMDzT-INCA	LSCE	00	Global
MACC	ECMWF	00	Global
MetUM	U. K. Met Office	00	Global
GEOS-5	NASA	00	Global
NGAC	NCEP	00	Global

VARIABLES: Dust surface concentration – Dust Optical Depth at 550 nm

LEAD TIME: 0 – 72 hours, every 3 hours

GEOGRAPHICAL DOMAIN: 25°W – 60°E, 0 – 65°N

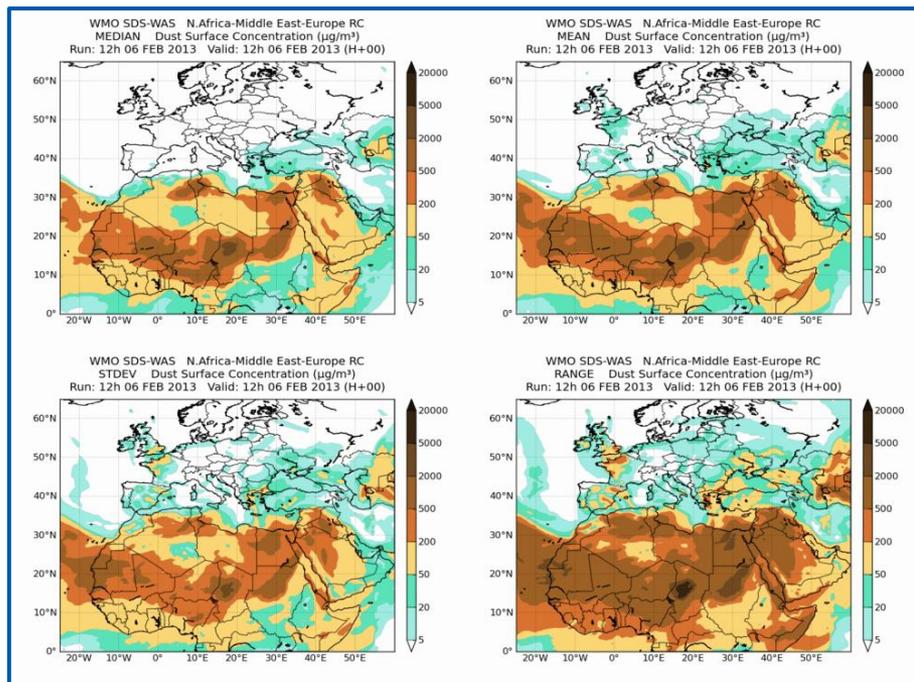
SDS-WAS RC: Joint visualization



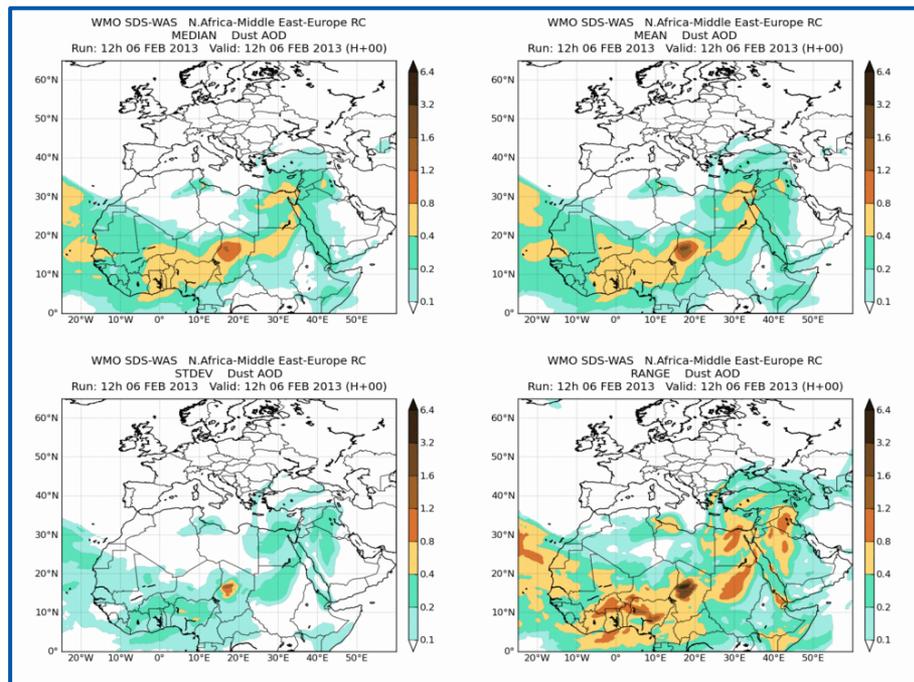
AOD at 550nm
from 6-Feb-2013 12:00 to
9-Feb-2013 00:00

SDS-WAS RC: Generation of multi-model products

Surface concentration



AOD at 550nm



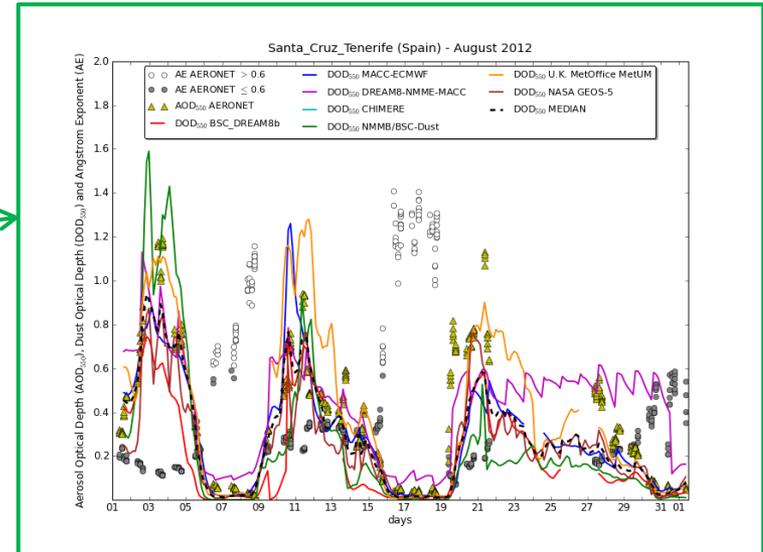
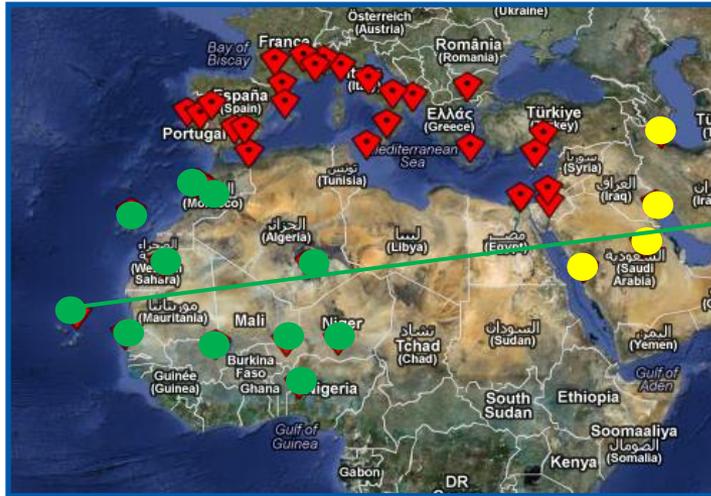
from 6-Feb-2013 12:00 to 9-Feb-2013 00:00

Model outputs are bi-linearly interpolated to a common $0.5^\circ \times 0.5^\circ$ grid mesh. Then, different multi-model products are generated:

CENTRALITY: median - mean

SPREAD: standard deviation – range of variation

SDS-WAS RC: NRT Evaluation using AERONET



Model evaluation metrics (bias, correlation, RMSE and FGE) are calculated:

- By regions: NA-ME-E, Sahel/Sahara, Middle East and Mediterranean
- By time periods: monthly, seasonal and annual

SDS-WAS RC: Forecast evaluation metrics

Dec 2012 - Feb 2013. Dust Optical Depth.

Threshold Angstrom Exponent = 0.600

BIAS

	BSC_ DREAM8b	MACC- ECMWF	DREAM8- NMME-MACC	NMMB/ BSC-Dust	U.K. Met Office	NASA GEOS-5	NCEP NGAC	MEDIAN
Sahel/Sahara <i>show stations</i>	-0.18	-0.14	-0.14	-0.09	0.00	-0.08	-0.03	-0.11
Middle East <i>show stations</i>	-0.12	-0.13	-0.04	-0.22	-0.00	-0.15	-0.14	-0.13
Mediterranean <i>show stations</i>	-0.13	-0.14	-0.12	-0.15	-0.09	-0.14	-0.11	-0.13
TOTAL	-0.16	-0.14	-0.13	-0.12	-0.03	-0.11	-0.07	-0.12

CORRELATION COEFFICIENT

	BSC_ DREAM8b	MACC- ECMWF	DREAM8- NMME-MACC	NMMB/ BSC-Dust	U.K. Met Office	NASA GEOS-5	NCEP NGAC	MEDIAN
Sahel/Sahara <i>show stations</i>	0.63	0.55	0.62	0.65	0.59	0.63	0.67	0.69
Middle East <i>show stations</i>	0.24	0.34	0.46	0.36	0.36	0.43	0.38	0.41
Mediterranean <i>show stations</i>	0.28	0.28	0.26	0.34	0.28	0.29	0.33	0.34
TOTAL	0.47	0.49	0.50	0.57	0.51	0.55	0.57	0.59

ROOT MEAN SQUARE ERROR

	BSC_ DREAM8b	MACC- ECMWF	DREAM8- NMME-MACC	NMMB/ BSC-Dust	U.K. Met Office	NASA GEOS-5	NCEP NGAC	MEDIAN
Sahel/Sahara <i>show stations</i>	0.31	0.29	0.28	0.25	0.24	0.25	0.22	0.25
Middle East <i>show stations</i>	0.28	0.27	0.23	0.31	0.24	0.27	0.26	0.26
Mediterranean <i>show stations</i>	0.27	0.27	0.28	0.27	0.27	0.28	0.26	0.27
TOTAL	0.29	0.28	0.28	0.27	0.25	0.26	0.24	0.26

FRACTIONAL GROSS ERROR

	BSC_ DREAM8b	MACC- ECMWF	DREAM8- NMME-MACC	NMMB/ BSC-Dust	U.K. Met Office	NASA GEOS-5	NCEP NGAC	MEDIAN
Sahel/Sahara <i>show stations</i>	0.89	0.84	0.74	0.88	0.64	0.70	0.59	0.65
Middle East <i>show stations</i>	0.67	0.74	0.53	1.14	0.47	0.73	0.67	0.61
Mediterranean <i>show stations</i>	1.45	1.52	1.23	1.64	1.22	1.52	1.19	1.40
TOTAL	1.07	1.07	0.90	1.18	0.83	1.00	0.82	0.92

- Besides dust, there might be other aerosol types (anthropogenic, biomass burning, etc.). Then, a small BE could be expected.
- Scores for individual sites can be little significant for being calculated from a small number of data.
- The RMSE is strongly dominated by the largest values. Especially in cases where prominent outliers occur, the usefulness of the RMSE is questionable and the interpretation becomes more difficult.

Applications of the model and ongoing work

Applications:

- ⌘ Generation of a reanalysis database of mineral dust aerosols
- ⌘ Applied for the study of the meningitis in central Africa
- ⌘ Providing mineral dust aerosol maps and vertical profiles for research studies
- ⌘ Contributing to SDS-WAS and ICAP model intercomparison initiatives

Ongoing work

- ⌘ Update of the reanalysis simulations
- ⌘ Improvements on the emission scheme
- ⌘ High resolution configurations



**Barcelona
Supercomputing
Center**

Centro Nacional de Supercomputación



SEA SALT AEROSOL MODULE

- ***main issues:***

- state-of-the-art models: errors of a factor of 2 or more on sea-salt AOD and SCONC monthly means
(Textor et al., ACP 2006; Kinne et al., ACP 2006)
- model uncertainties: mainly due to the parameterization of sea-salt emission (approach, parameters, validity size range, production mechanisms, etc.)

- ***guidelines:***

- keeping the NMMB/BSC-CTM general philosophy i.e. introducing “complexity” only when necessary
- embedded implementation within NMMB
(aerosol-meteo on-line coupling)
- short/medium term forecast of aerosol AOD and surface concentrations, not CCNs prediction

- ***and assumptions:***

- sea-salt (SS) externally mixed with dust (DU)
- prognostic variables: 8 bins (dry mass mixing-ratios)
- bins range from $0.1\mu\text{m}$ to $15\mu\text{m}$ in dry radius (ultrafine particles not considered)
- water aerosol implicitly described by the water-uptake, not included as a prognostic specie
- water-uptake only affects removal/vertical-oriented processes, not the horizontal transport
- surf-zone production not considered in this work

SEA-SALT MODULE (emissions)

$$dF/dr = f(r, \xi)$$

M86 → $\xi = U_{10}$ (bubbles)

G03 → $\xi = U_{10}$ (bubbles, spume?)

M86/SM93 → $\xi = U_{10}, U_T=9\text{m/s}$ (bubbles, spume)

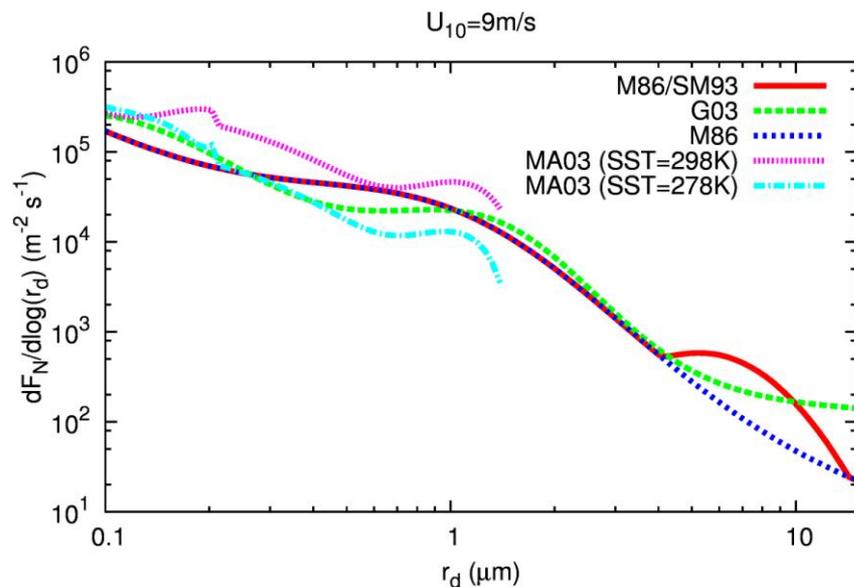
M86/SM93/MA03 → $\xi = (U_{10}, U_T, \text{SST})$ (bubb., sp.)

Monahan et al. (OW 1986)

Gong et al. (GBC 2003)

Smith et al. (RMS/QJ 1993)

Martensson et al. (JGR 2003)



criteria:

- whitecap method
- simplest (low number of parameters)
- bubbles and spume mechanisms

(M86 and G03 extended up to 15 μm)

→ **strong differences**
for $r_d > 5\mu\text{m}$ (spume)
and for $0.1\mu\text{m} < r_d < 1\mu\text{m}$ (bubbles)

SEA-SALT MODULE (water uptake and other processes)

- aerosol module extended to wet aerosol
- simplified parameterization of hygroscopic growth (Chin et al., JGR 2002)

RH(%)	ϕ
< 50	1.0
50 – 70	1.6
70 – 80	1.8
80 – 90	2.0
90 – 95	2.4
95 – 99	2.9
> 99	4.8

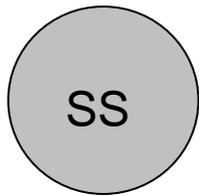
$$r_d \rightarrow r_w = r_d \cdot \Phi(\text{RH})$$

$$\rho_d \rightarrow \rho_w = \rho_d \Phi^{-3} + (1 - \Phi^{-3}) \rho_{\text{water}}$$

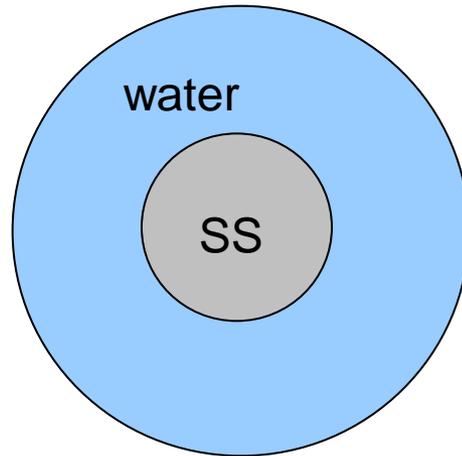
(...)

DRY BINS:

- hor. transport
- emissions



r_d



r_w

WET BINS:

- **dry dep. + sedimentation** (Zhang et al., AE 2001)
- **in-cloud and below-cloud scavenging:**
 - **grid-scale clouds** (Slinn, 1984)
coupled with the new Ferrier microphysics
 - **sub-grid clouds** (Pérez et al., ACP 2011)
coupled with the Betts-Miller-Janjic (BMJ) adjustment scheme of NMMB
- **optical properties**

2006 annual simulation
(reference year)
6h-output

GLOB(L) → 1.4deg x 1deg

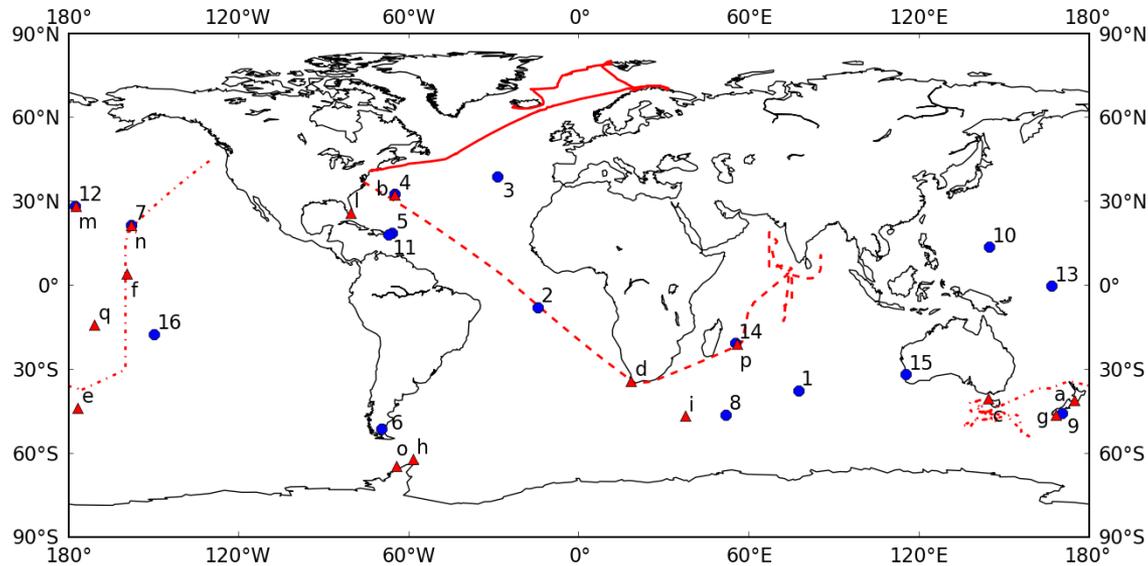
GLOB(H) → 0.465deg x 0.333deg

REG → 0.1deg x 0.1deg

(New Zealand, Marion Island, ...)

- *GFDL radiative scheme (no feedbacks)*
- *ICs → FNL (year > 1999) or GDAS (year ≤ 1999)*
- *NO REG Bcs → large domains*
- *24h-simulations covering the whole temporal interval*

SEA-SALT MODULE (observational networks)



Optical depth (AOD_{500nm})

● AERONET stations

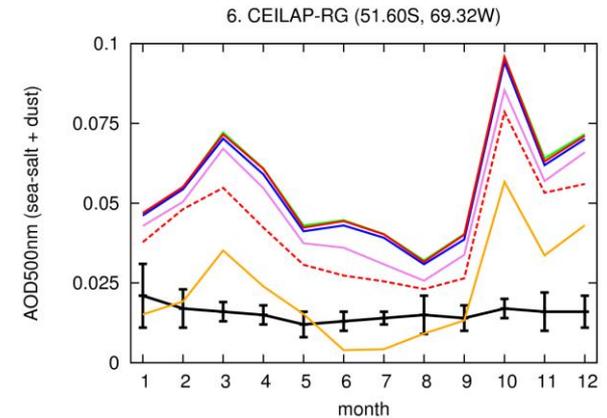
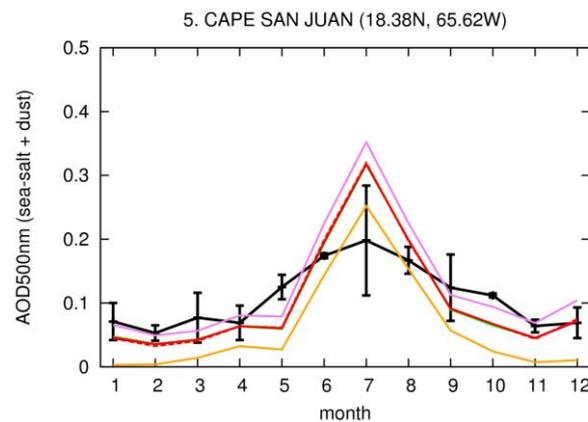
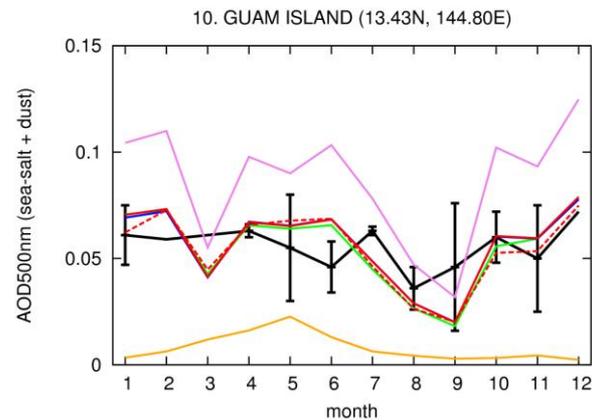
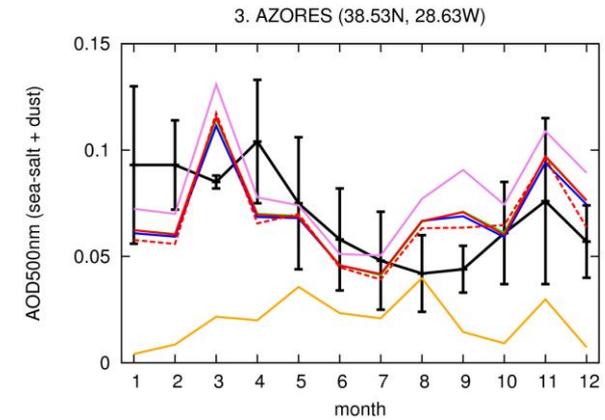
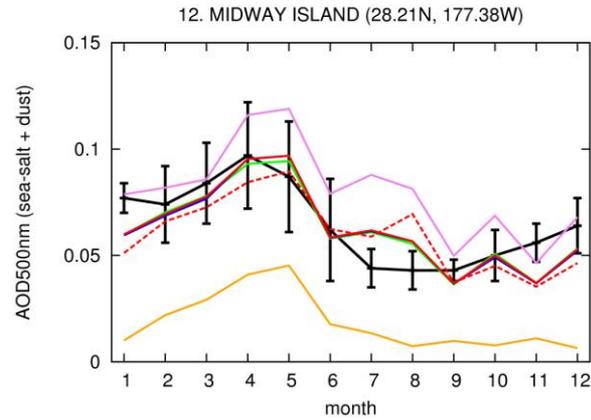
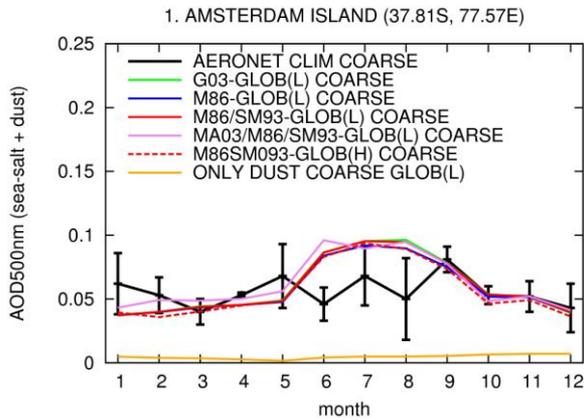
(stations with a sea-salt contribution to the total AOD > 50%, following Jaegle et al., 2011)

Surface concentrations (SCONC):

▲ U-MIAMI network

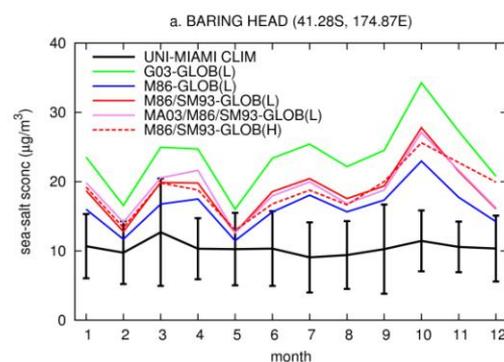
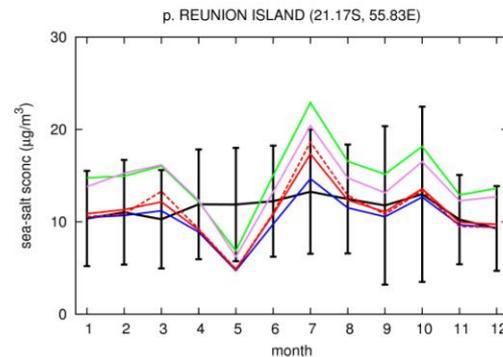
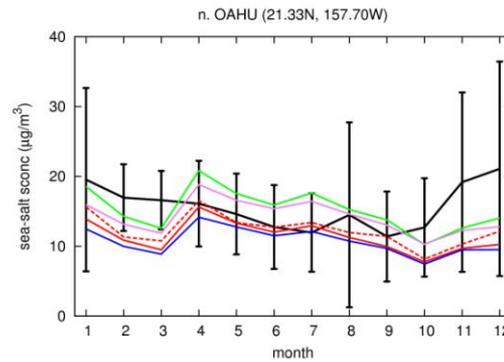
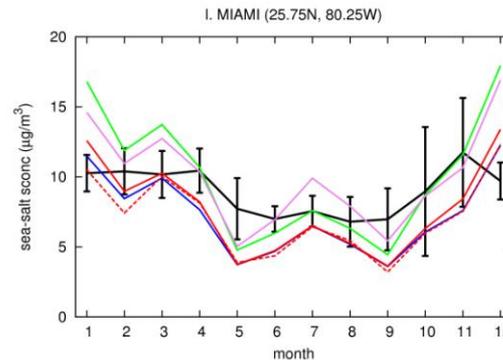
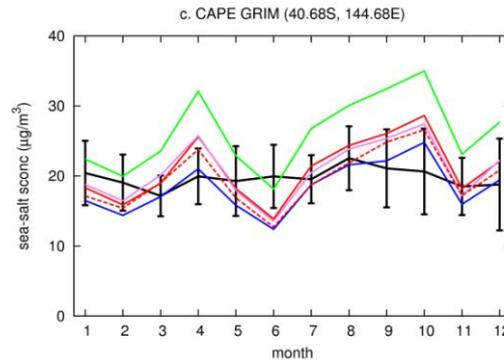
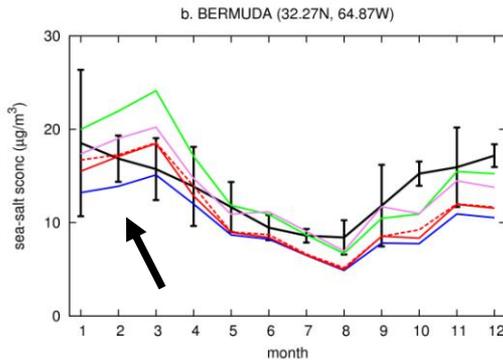
▤ NOAA/PMEL cruises (ICEALOT, AEROINDO, ACE1)

SEA-SALT MODULE (results: COARSE AOD500nm)



→ **DU** may strongly influence some “sea-salt characterized” stations

SEA-SALT MODULE (results: SURFACE CONC)

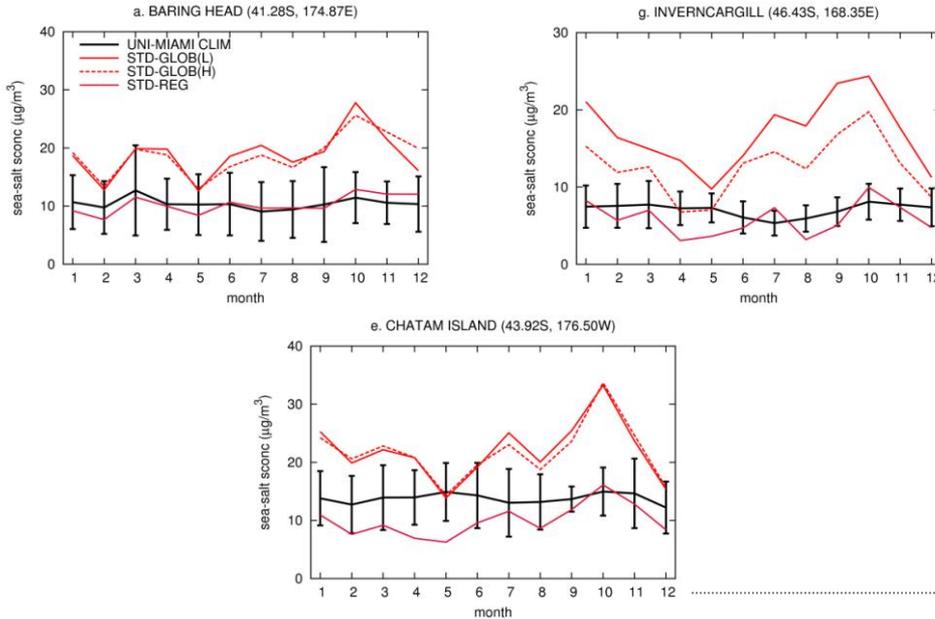


- relevant differences among schemes
- extended **G03** too high (due to its spume production)
- **M86** vs **M86/SM93**: spume contribution may affect monthly means in specific sites and months (for ex. Bermuda in JFM)

→ since its overall performance in simulating **AOD and SCONC** we assume **M86/SM93** as default emission scheme

SEA-SALT MODULE (results: SURFACE CONC / REG)

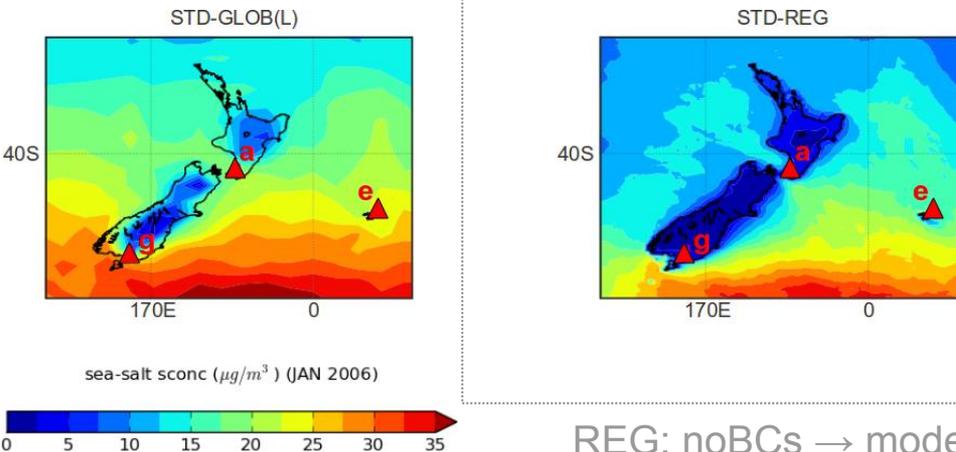
- GLOB(L) and GLOB(H) resolutions seem to give quite similar results, although...



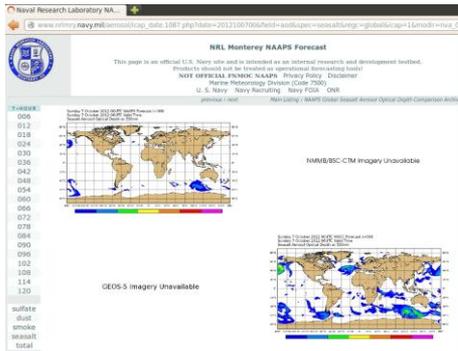
→ at smaller scales
(REG = 0.1 x 0.1)
the model becomes able to
resolve steep topographies

→ in these cases (such as
for the New Zealand domain),
the observed SCONC
climatologies are reproduced

→ obvious but not trivial:
smaller scales (≈ 0.1 deg)
effects may affect
larger scales (> 1 deg)

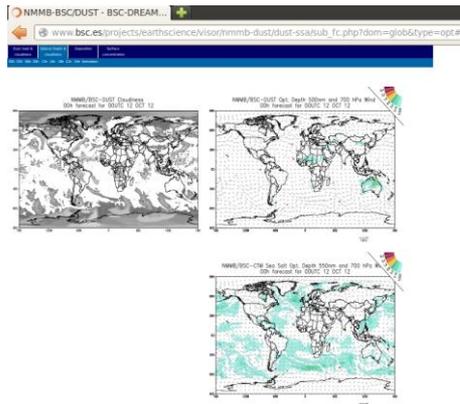


REG: noBCs → model domain boundaries far from the region in study



- participate in the ICAP model intercomparison project

<http://www.nrlmry.navy.mil/aerosol/icap.1087.php>



- include the sea-salt module in the BSC operational aerosol forecast (dust already available)

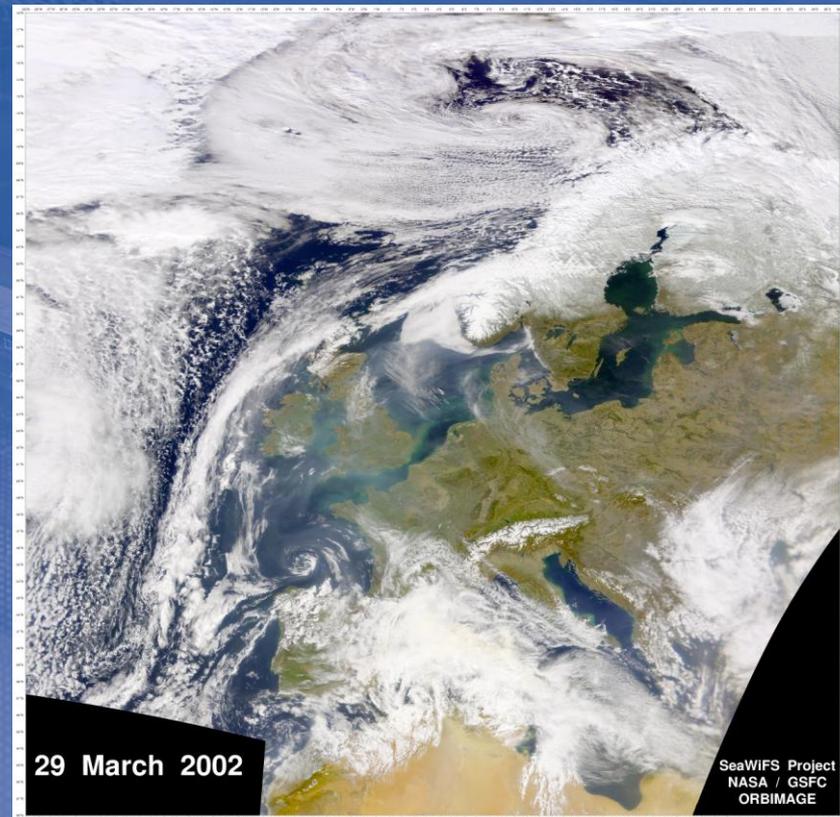
<http://www.bsc.es/earth-sciences/mineral-dust/nmmbbsc-dust-forecast>

- carry on the development of the complete aerosol module (DU, SS, BC, OC, SO₄)



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29 March 2002

SeaWiFS Project
NASA / GSFC
ORBIMAGE

GAS-PHASE MODULE

Photolysis scheme

- 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-CTM 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 $\Phi_i(\lambda)$ to be updated from Prather Fast-JX.

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 pre-processor (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
- Stratospheric ozone: linear model Cariolle and Teysse re (2007) or Monge-Sanz et al. (2011)

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 deposition and vertical diffusion at first model level at same time.

$$dC_i(z_{ref})/dt = -V_d(z_{ref}) \times C_i(z_{ref})/\Delta z$$

$$V_d = (R_a + R_b + R_c)^{-1}$$



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:

$$\left. \frac{\partial \bar{m}_i}{\partial t} \right|_{cld} = \left. \frac{\partial \bar{m}_i}{\partial t} \right|_{subcld} + \left. \frac{\partial \bar{m}_i}{\partial t} \right|_{rescld}$$

$$\left. \frac{\partial \bar{m}_i}{\partial t} \right|_{scav} = \frac{-cld}{m_i} \left(\frac{e^{-\alpha_i \tau_{cld}} - 1}{\tau_{cld}} \right)$$

- Wet deposition:

$$wdep_i = \int_0^{\tau_{cld}} \frac{-cld}{m_i} P_r dt$$

$$\alpha_i = \frac{1}{\tau_{washout} \left(1 + \frac{TWF}{H_i} \right)}$$

$$\tau_{washout} = \frac{\bar{W}_T \Delta z_{cld}}{\rho_{H_2O} P_r}$$

$$TWF = \frac{\rho_{H_2O}}{\bar{W}_T R T}$$

The NMMB/BSC-CTM: Model configuration

Global configuration:

- Global domain at $1.4^\circ \times 1^\circ$ horizontal resolution
- 24 vertical levels
- Nonhydrostatic dynamics
- Initial conditions from NCEP/FNL meteorological analysis $1 \times 1^\circ$
- Anthr. emissions: ACCMIP
- Biogenic emissions: MEGANv2 on-line
- Strat. Ozone: COPCAT
 - *Annual simulation: 2004*

Regional configuration:

- European domain at $12\text{km} \times 12\text{km}$ horizontal spatial resolution
- 24 vertical layers
- Nonhydrostatic dynamics
- Initial conditions from NCEP/FNL meteorological analysis $1 \times 1^\circ$ and BC every 6h
- Anthr. Emissions: EMEP-HERMES
- Biogenic emissions: MEGANv2 on-line
- Chemical BC from global run
 - *Summer 2004*

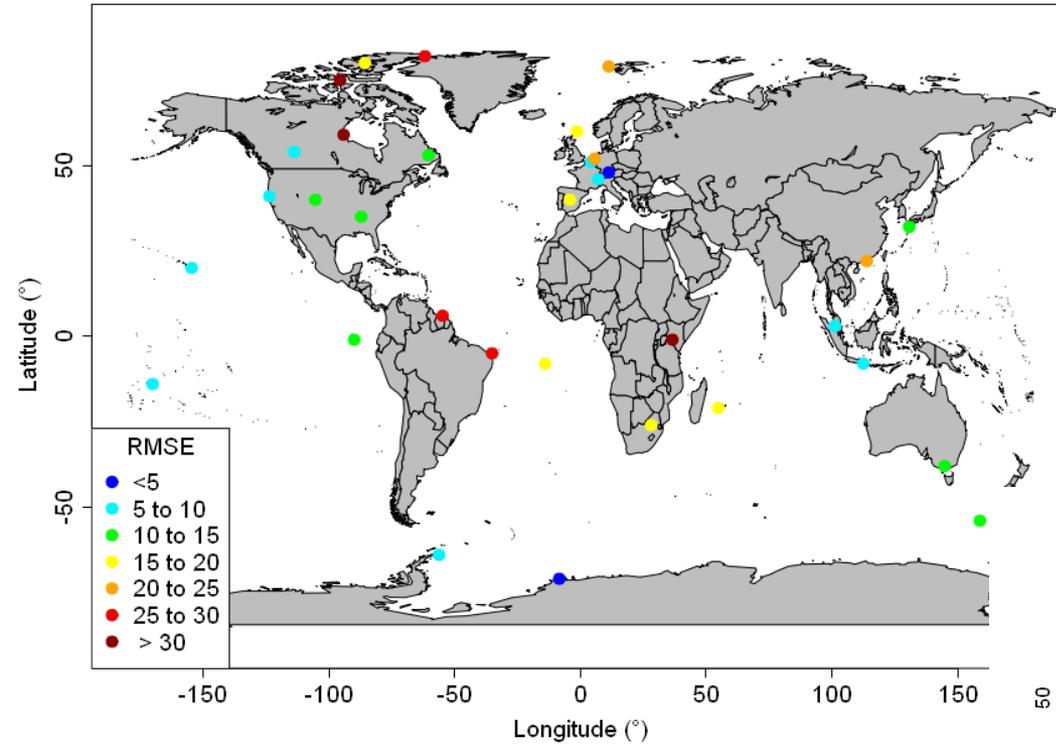
Evaluation of global and regional runs

- Surface O_3 , NO_2 , CO
- O_3 Vertical profiles: ozonesondes, HALOE

Ozonesondes (WOUDC, CMD and SHADOZ) - RMSE (monthly data)

TROPO

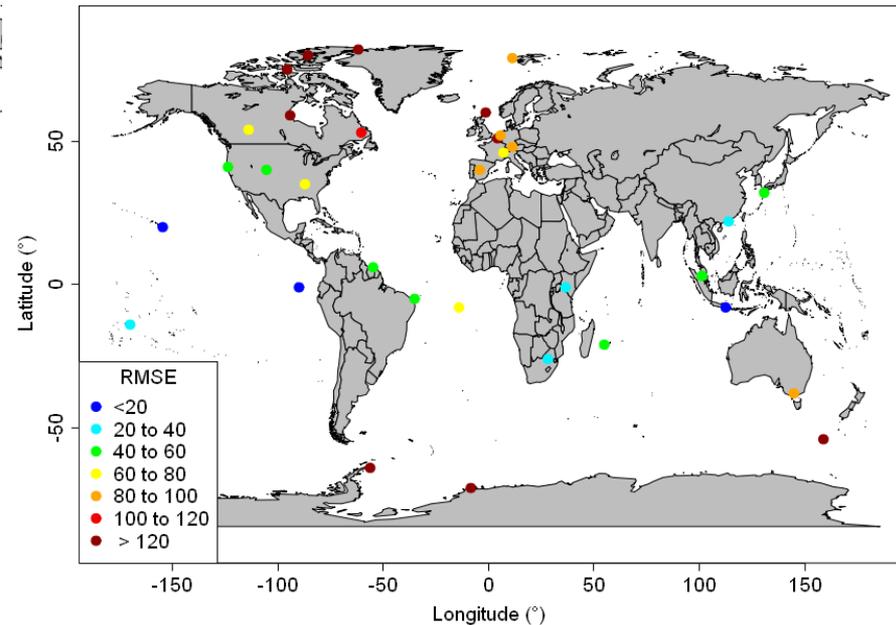
Root Mean Square Error(ppbv) for every station in the troposphere layer(10000m<)(ppbv)



Mean RMSE
July-August 2004

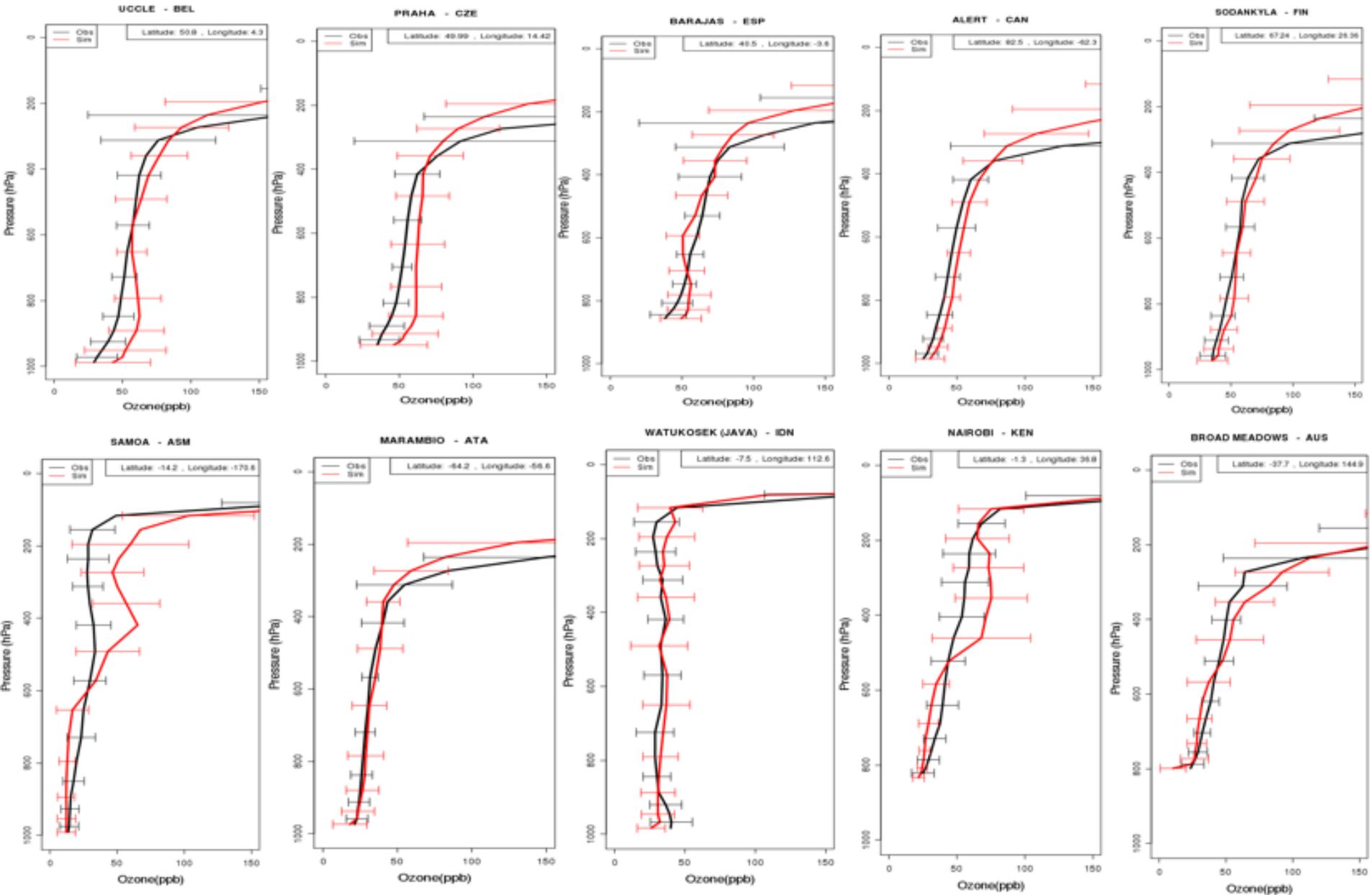
lower STRATO

Root Mean Square Error(ppbv) for every station in the stratosphere layer(10000m>)(ppbv)



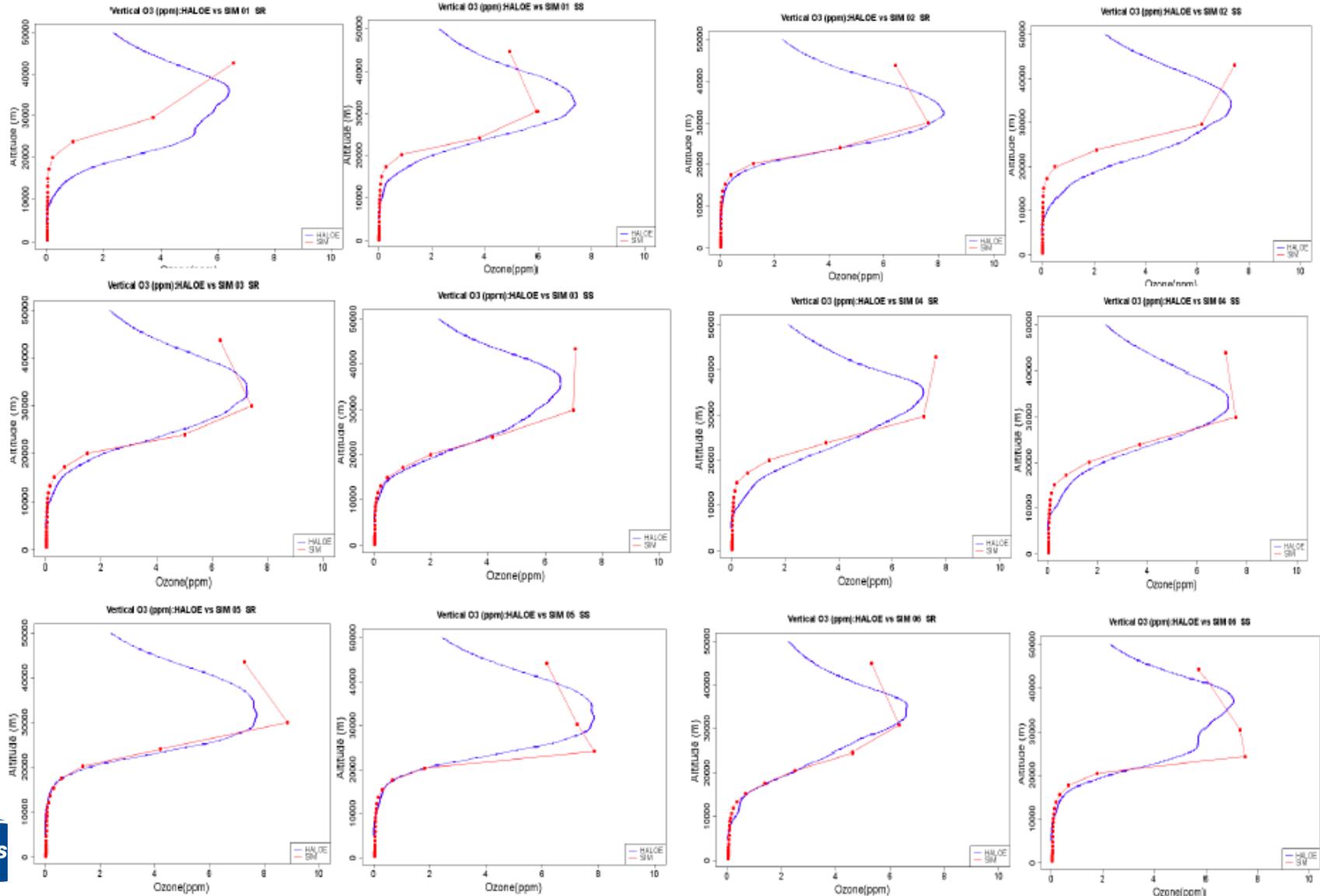
VERTICAL PROFILES (PPB)	MEAN TROPO (<10000m)	MEAN LOW STRATO (10000-18000)
OBS WOULD	50.89	344.976
SIM COPCAT	43.42	363.63

Ozone profile from ozonesondes



Ozone profile from HALOE retrievals

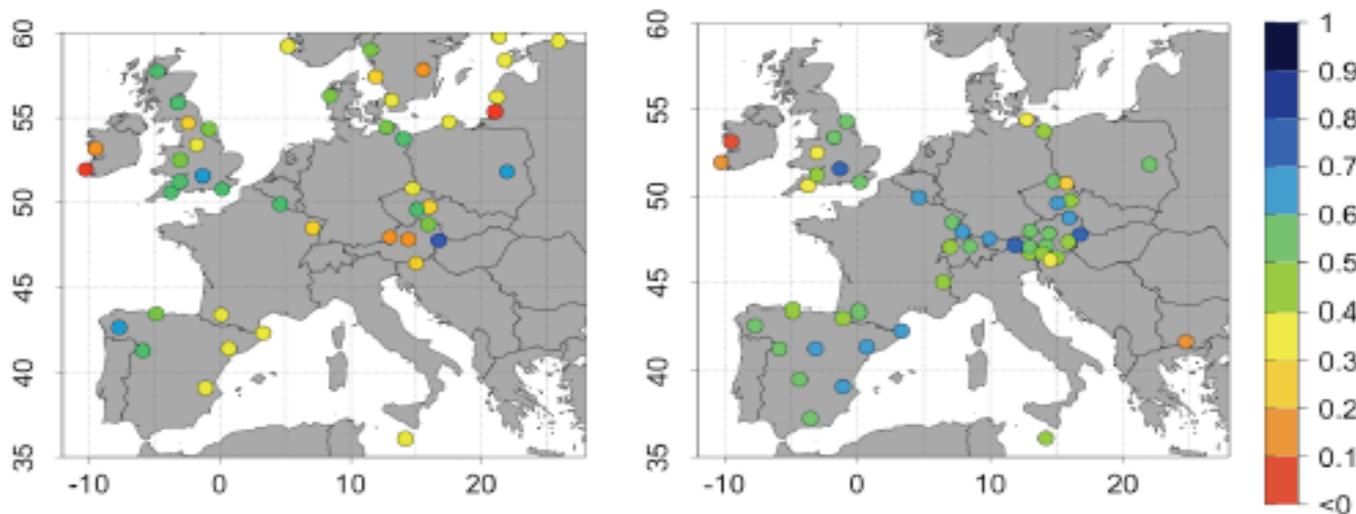
HALOE 2004 month 1-6



Coupled global (1°) to regional (12 km) run

Results for August months for global and regional runs – EMEP background stations

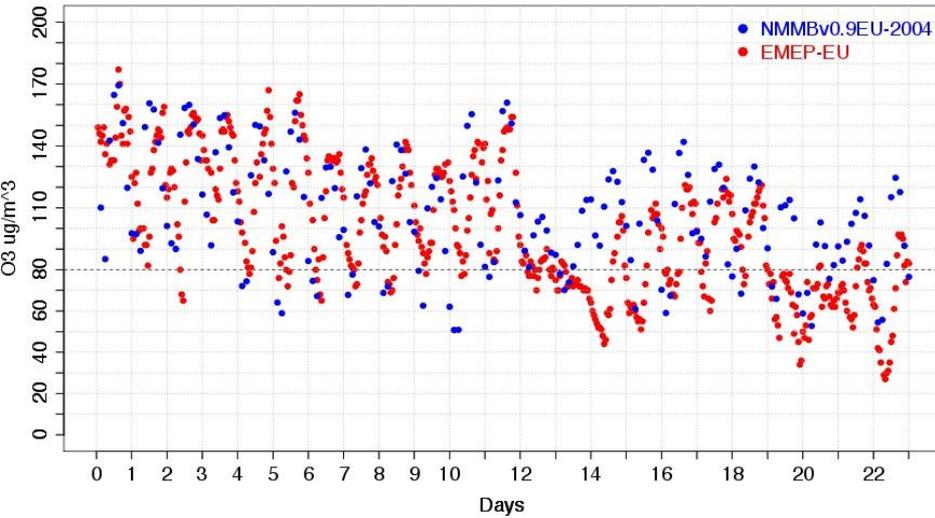
Run	Corr.	MB ($\mu\text{g}/\text{m}^3$)	RMSE ($\mu\text{g}/\text{m}^3$)	MNBE (%)	MNGE (%)	MFB (%)	MFE (%)
Global	0.33	-12.9	41.4	-11.5	30.9	-21.3	36.7
Regional	0.51	0.7	23.1	2.1	17.2	-0.3	17.1



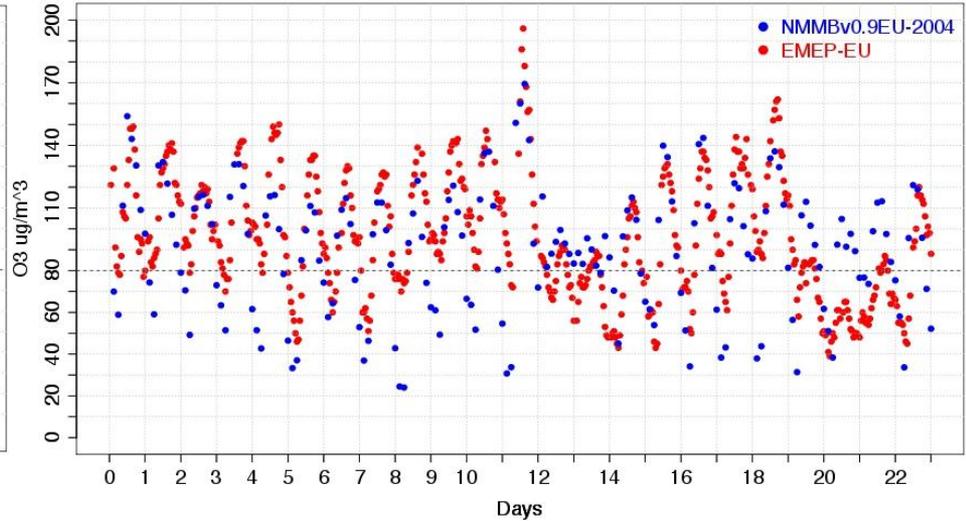
Surface ozone correlation at several EMEP stations – Global (left) and Regional (right)

Regional run: Model vs Obs

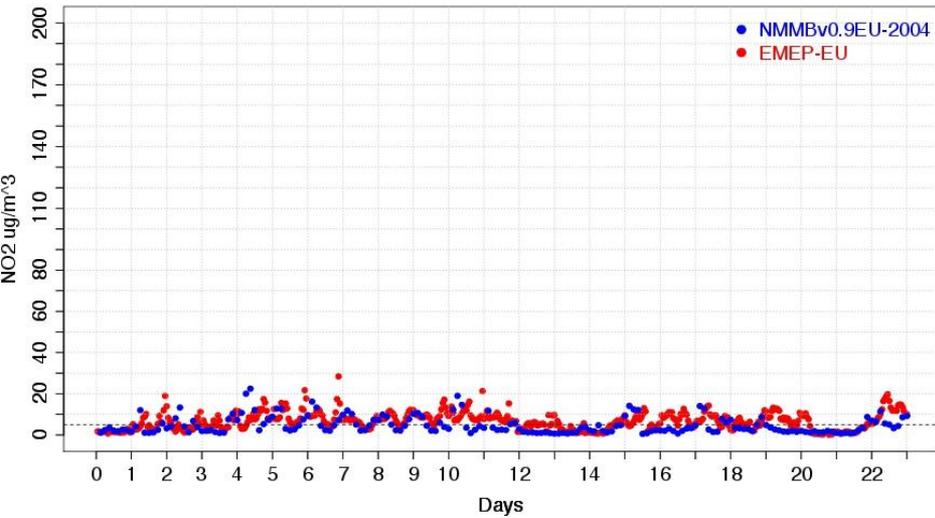
O3 - NMMBv0.9EU-2004 - EMEP-EU - Austria_Haunsberg_AT41 - Year: 2004 - Julian days: from 214 to 228



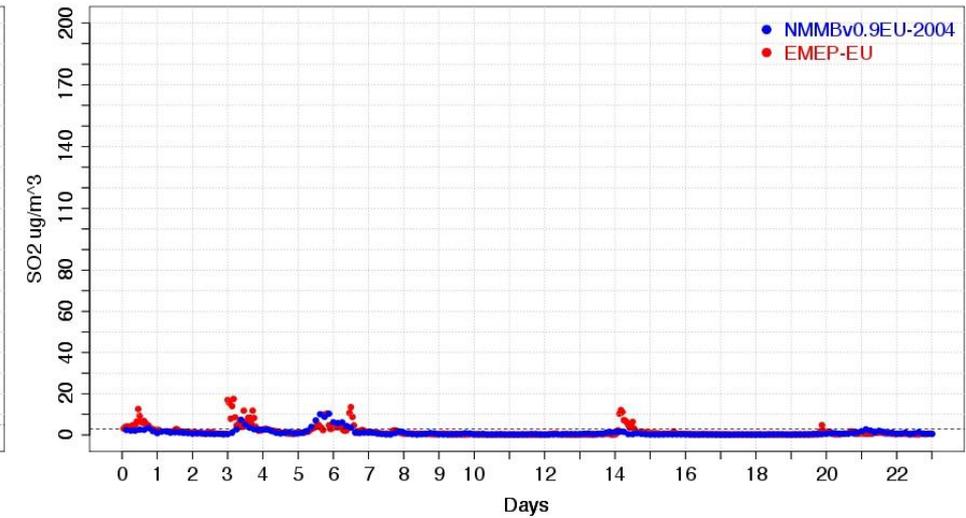
O3 - NMMBv0.9EU-2004 - EMEP-EU - Austria_Pillersdorf_AT30 - Year: 2004 - Julian days: from 214 to 228



NO2 - NMMBv0.9EU-2004 - EMEP-EU - Netherlands_Kollumerwaar_NL09 - Year: 2004 - Julian days: from 214 to 228



SO2 - NMMBv0.9EU-2004 - EMEP-EU - Spain_O_Savinao_ES16 - Year: 2004 - Julian days: from 214 to 228



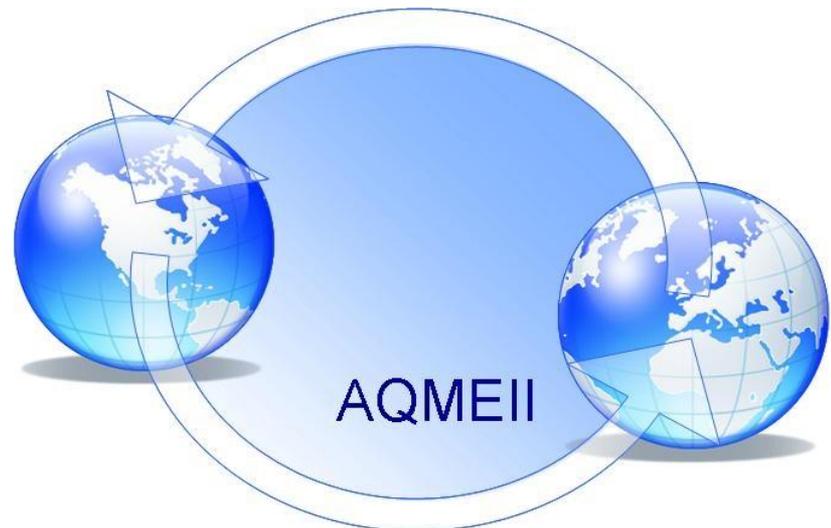
Participating in AQMEII-Phase 2

⌘ AQMEII – Air Quality Modelling Evaluation International Initiative

⌘ Phase 2 – Regional on-line Air Quality Models

- Common domain: EU $0.22^{\circ} \times 0.22^{\circ}$
- Common anthropogenic emissions: TNO for Europe
- Common chemical BC: MACC

⌘ Contributing in the European runs with NMMB/BSC-CTM regional configuration



Model configuration

Period: Run one year simulation (2010).

Domain: European simulations: 30W- 60E, 25N-70N

Chemical BC: MACC (IFS-MOZART)

Meteorological BC: GFS

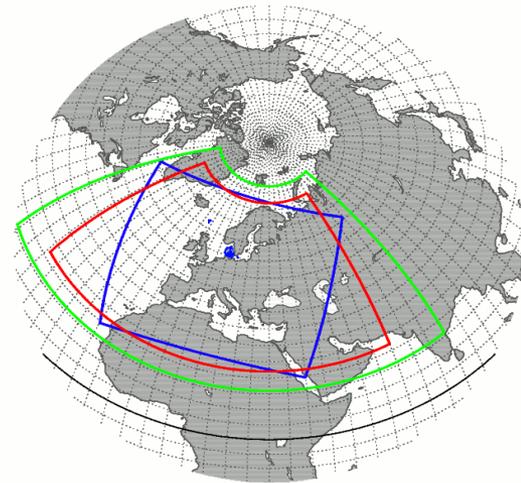
Emissions: TNO-MACC; Biogenics: MEGAN

Horizontal Resolution: $0.2^\circ \times 0.2^\circ$

Vertical Resolution: 24 top 50hPa

Chemical mechanism: CB05

Aerosols: only dust-ssa



Blue: model domain

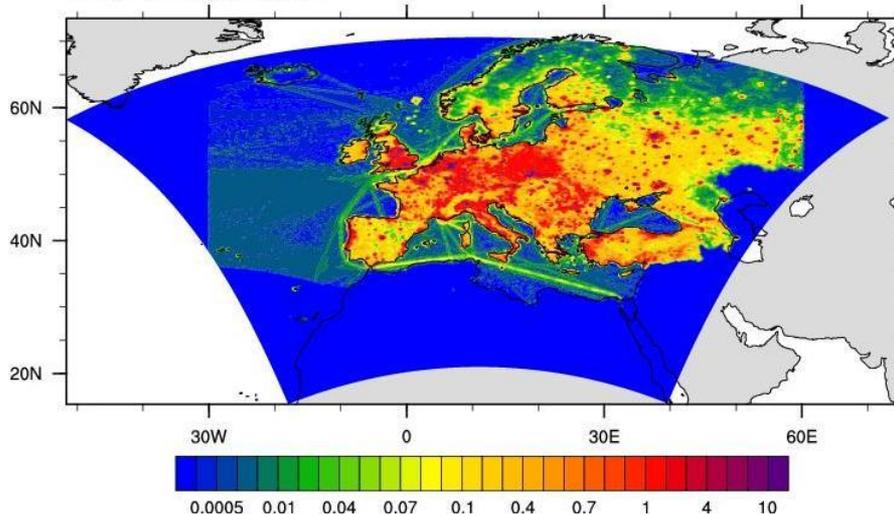
Red: AQMEII domain (to submit)

Green: BC domain

Anthropogenic emissions TNO (kg/(km² h))

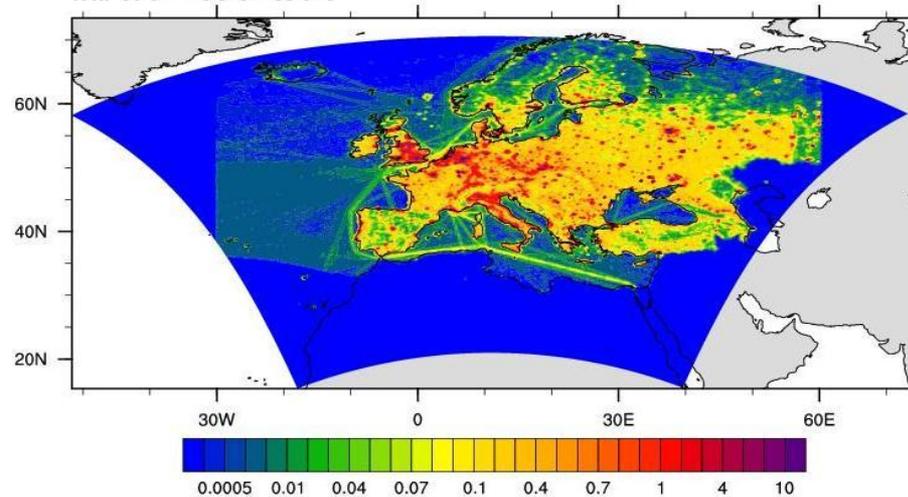
NMMB/BSC-CTM 20100101 12 UTC - AQMEII2 domain

total column CO emissions



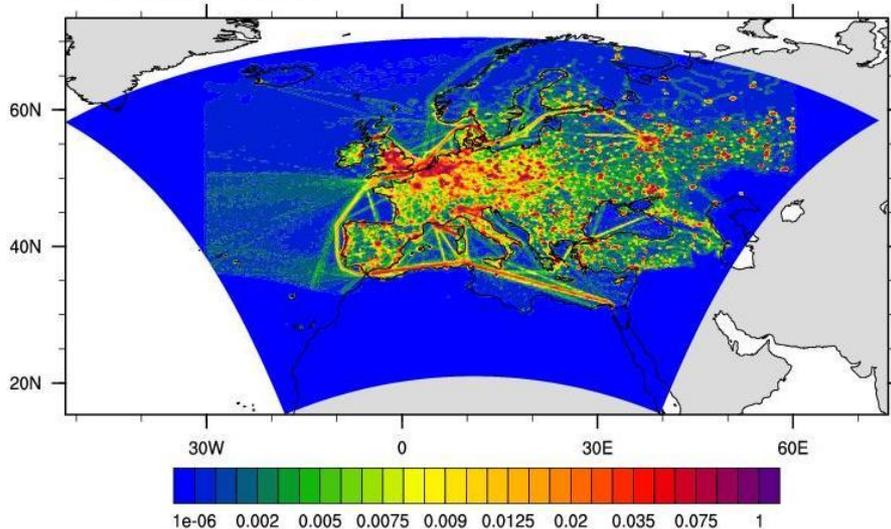
NMMB/BSC-CTM 20100701 12 UTC - AQMEII2 domain

total column CO emissions



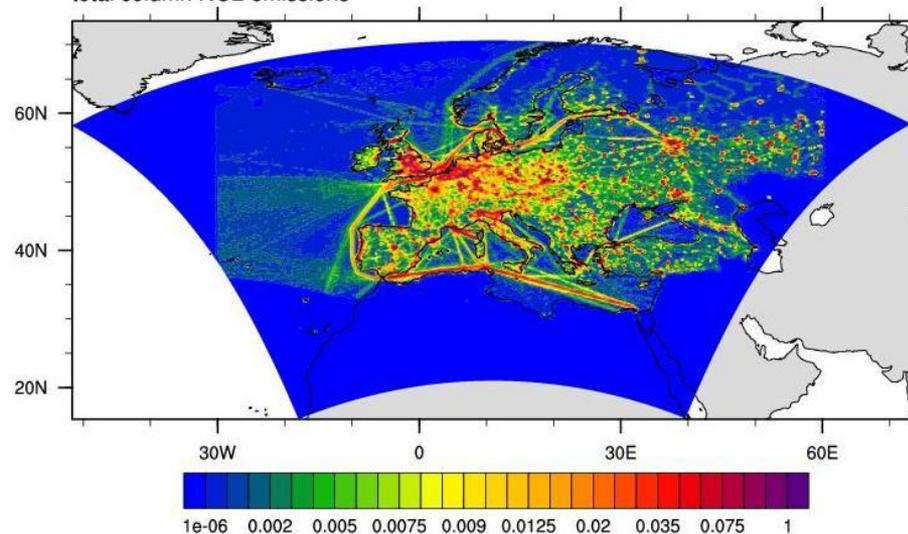
NMMB/BSC-CTM 20100101 12 UTC - AQMEII2 domain

total column NO₂ emissions



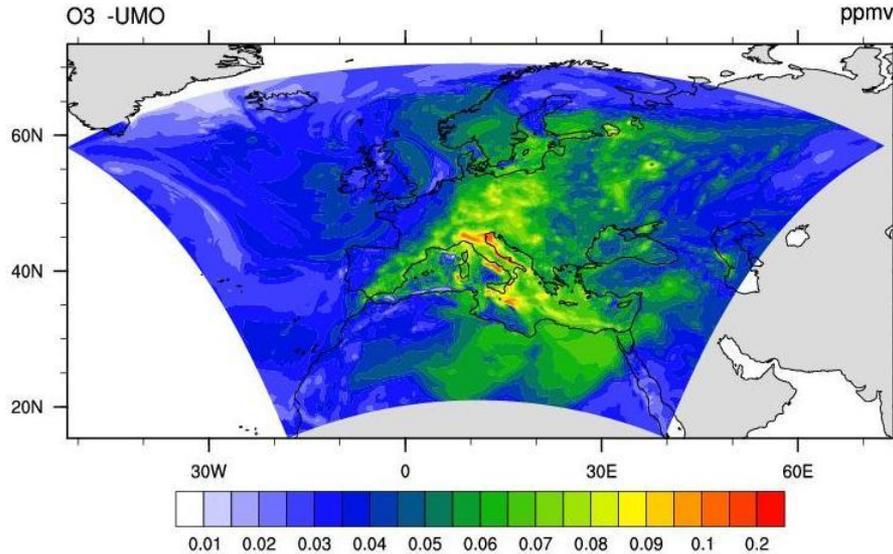
NMMB/BSC-CTM 20100701 12 UTC - AQMEII2 domain

total column NO₂ emissions

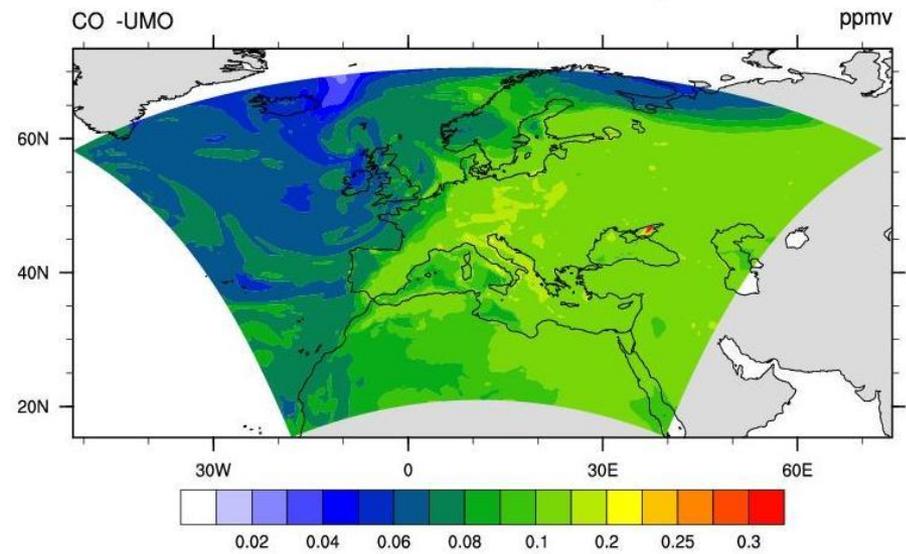


SURFACE concentration over the whole domain

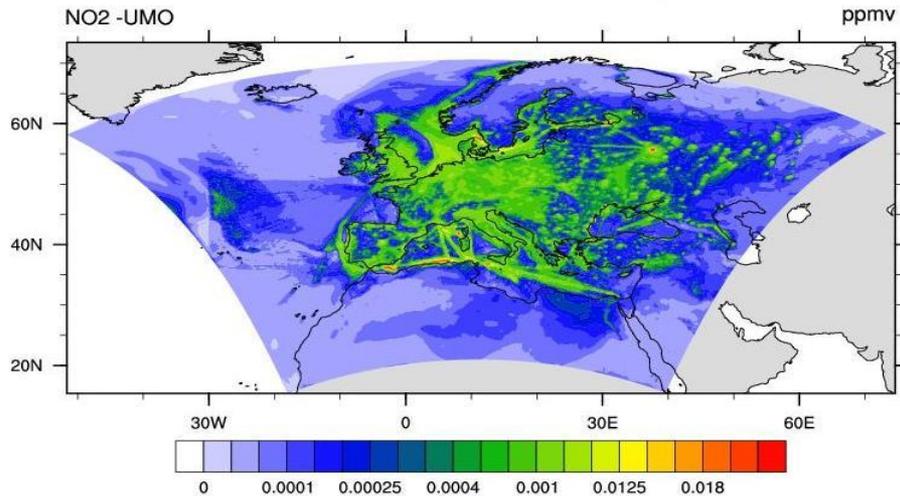
NMMB/BSC-CTM 20100715 12 UTC - AQMEII2 domain



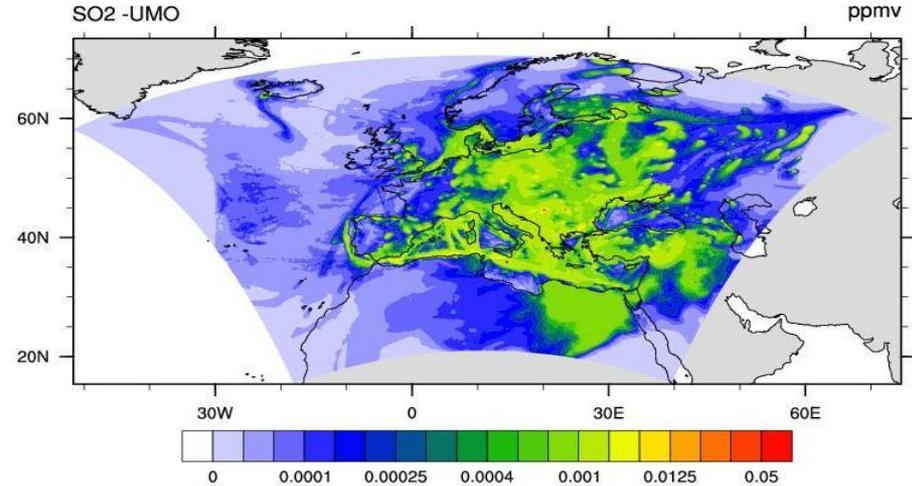
NMMB/BSC-CTM 20100715 12 UTC - AQMEII2 domain



NMMB/BSC-CTM 20100715 12 UTC - AQMEII2 domain

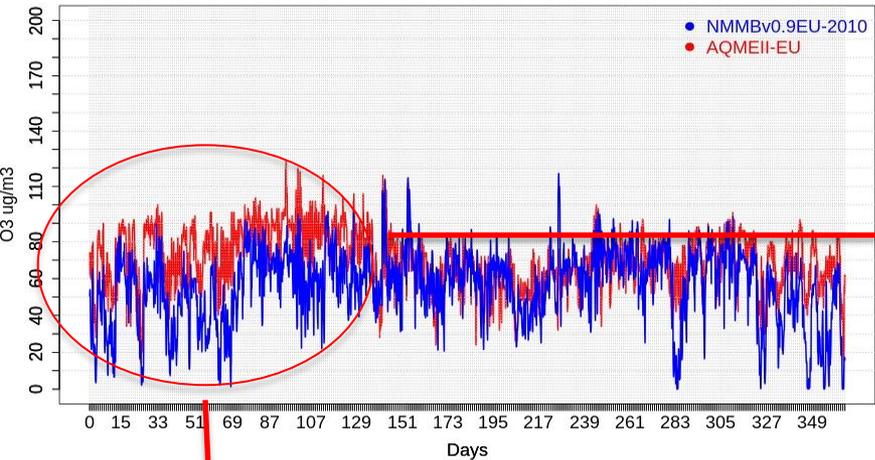


NMMB/BSC-CTM 20100715 12 UTC - AQMEII2 domain

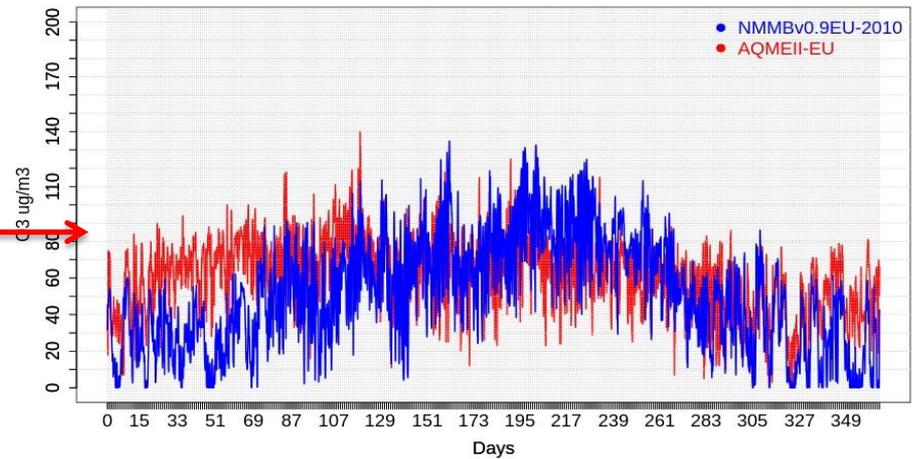


Preliminary results: Model vs Observations (surface O3)

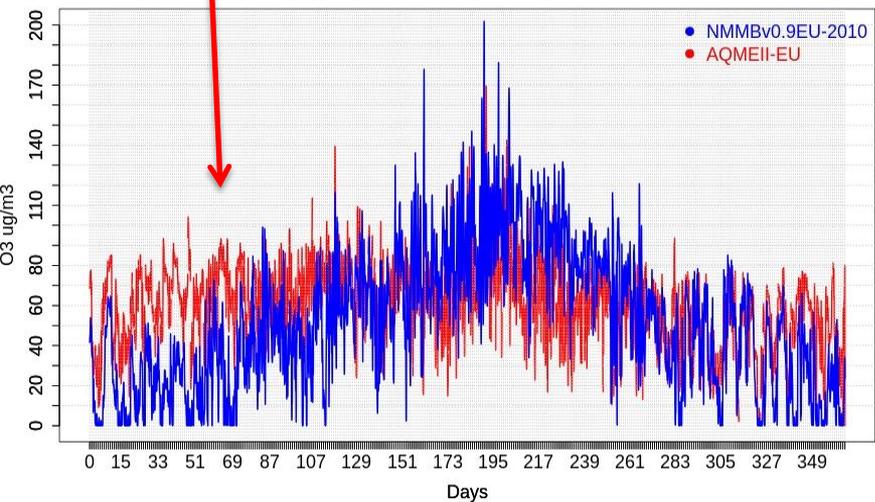
O3 - Mace_Head - Lat=53.1 Lon=-9.3 - R=0.52 RMSE=22.46 BIAS=-14.1



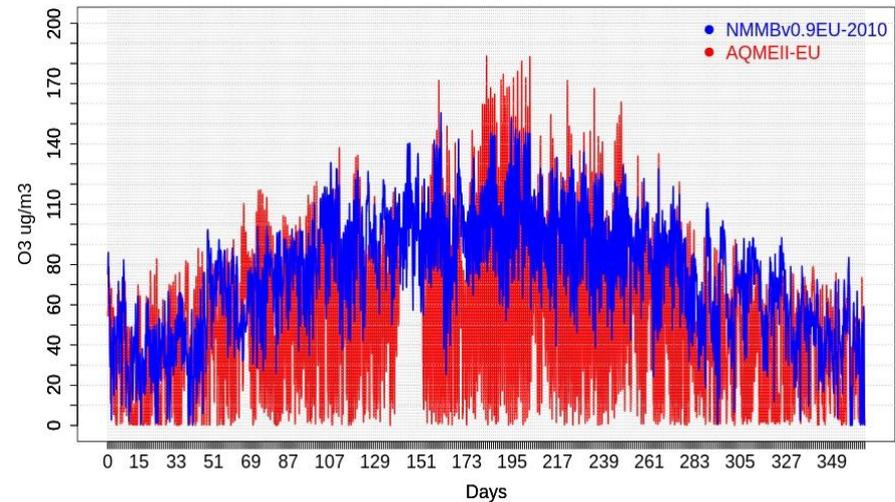
O3 - Leba - Lat=54.46 Lon=17.32 - R=0.53 RMSE=27.53 BIAS=-10.21



O3 - Zingst - Lat=54.26 Lon=12.44 - R=0.5 RMSE=31.17 BIAS=-9.07

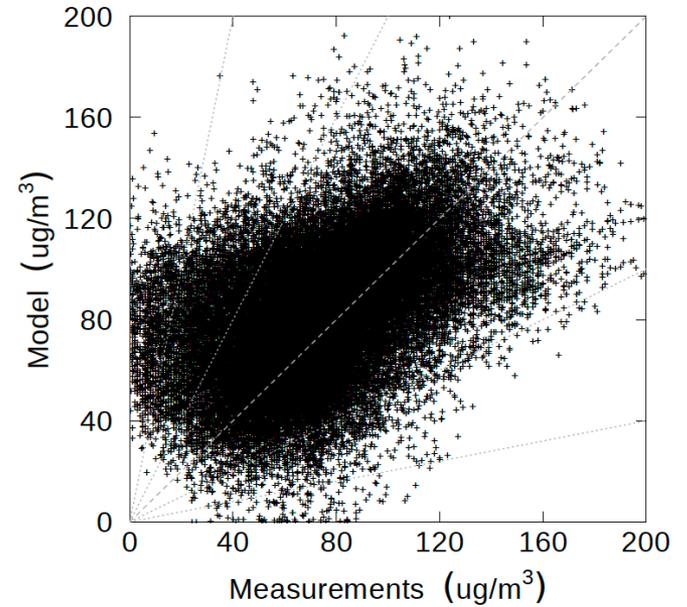
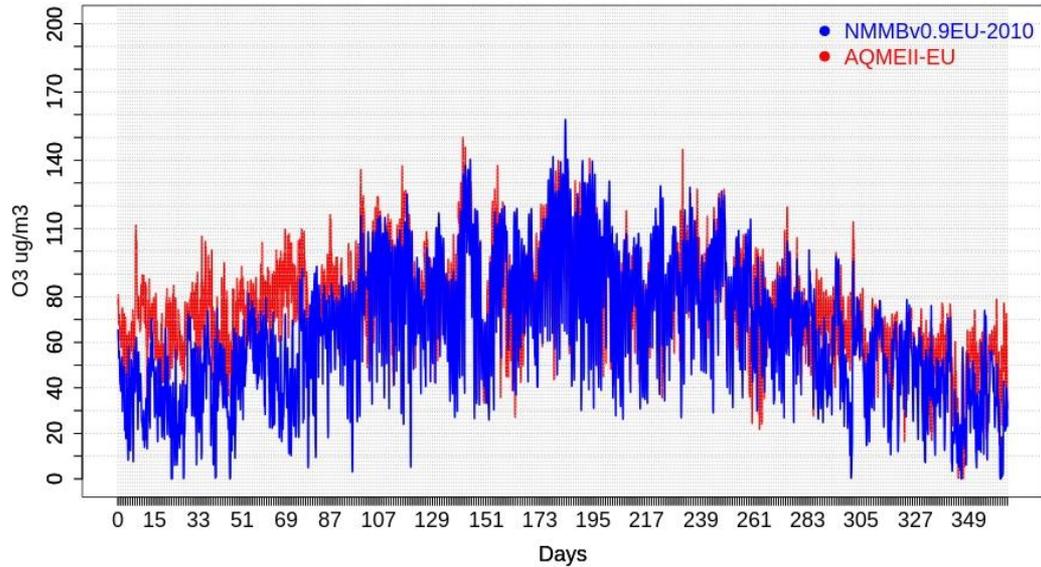


O3 - Montelibretti - Lat=42.6 Lon=12.38 - R=0.57 RMSE=39.64 BIAS=24.29

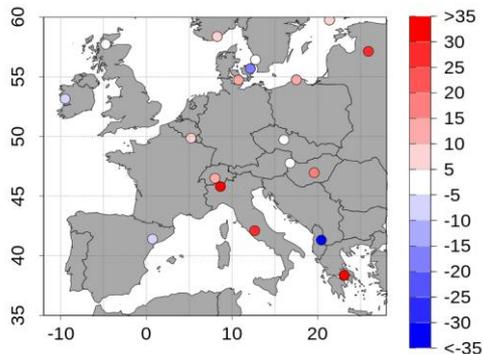


MODEL vs OBSERVATIONS (surface O3)

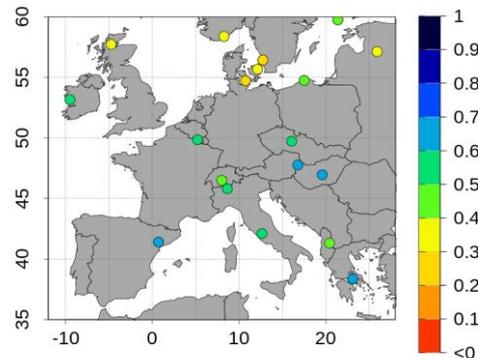
O3 - Els_Torms - Lat=41.24 Lon=0.43 - R=0.7 RMSE=23.88 BIAS=-11.39



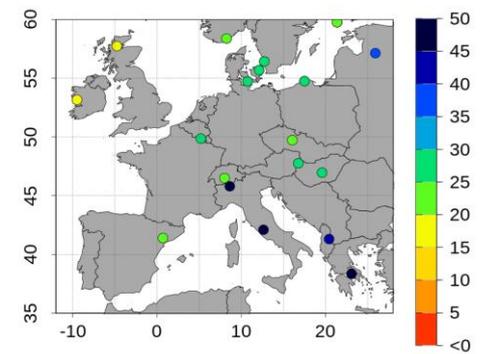
BIAS



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RMSE





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FUTURE WORK

Future Developments

- ⌘ Upgrade the meteorological driver to NEMS/NMMB 2013 version
- ⌘ Coupling of chemistry gas-phase with a secondary aerosol scheme for LAM applications at high-resolutions.
- ⌘ Implementation of the other global relevant aerosol species, i.e. black (BC) and organic carbon (OC), and sulfate (SO₄), in addition to dust (DU) and sea salt (SSA).
- ⌘ Implementation of a volcanic ash module (Fall3D model, Folch et al., 2008) within the modeling system
- ⌘ Implement radiative effects of aerosols
- ⌘ Explore methodologies for aerosol data assimilation

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Thank you!

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