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EXCELENCIA SEVERO OCHOA

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

Atmospheric chemistry studies with the NMMB/BSC-CTM model at the Barcelona Supercomputing Center

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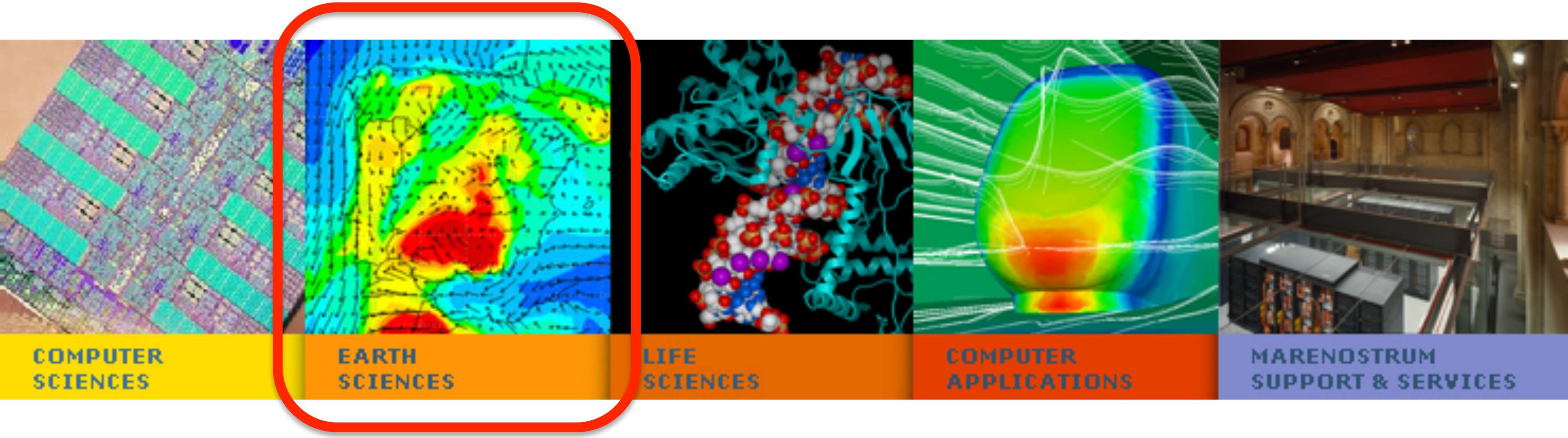
Contributions: Z. Janjic, S. Basart, A. Badia, M. Spada, J.M. Baldasano, E. DiTomaso, G.S. Markomanolis, K. Serradell, D. Dabdub, C. Pérez, K. Haustein, T. Black, A. Folch, A. Martí

NCEP/EMC Seminar, Maryland, April 16, 2014

The BSC-CNS (www.bsc.es)



The Earth Sciences Department is devoted to the development and implementation of regional and global state-of-the-art models for air quality, meteorology and climate applications

Earth Sciences Activities

- Research lines:
  - Air Quality
  - Mineral Dust
  - Atmospheric Modeling
  - Climate Modeling
- New on-line Meteorology-Chemistry model:
  - **NMMB/BSC-CTM**
- Dust daily forecast:
  - **BSC-DREAM8b**

    http://www.bsc.es/projects/earthscience/BSC-DREAM/
  - **NMMB/BSC-Dust:**

    http://www.bsc.es/projects/earthscience/NMMB-BSC-DUST/
  - **Mineral dust database:** Files download

    http://www.bsc.es/earth-sciences/mineral-dust/catalogo-datos-dust/

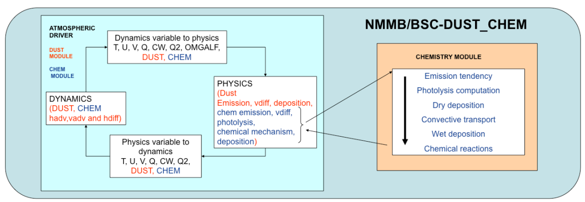
NMMB/BSC-Chemical Transport Model (Overview)

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

NMMB/ BSC-CTM

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

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



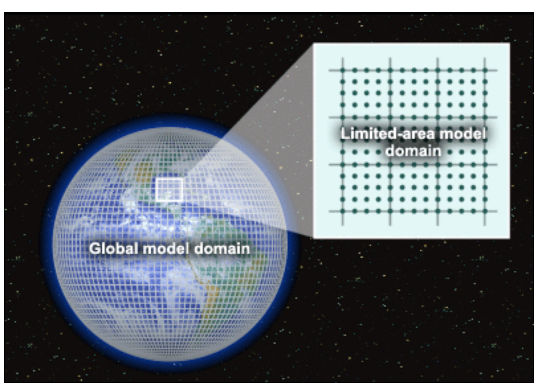
BSC Chemical Transport Model
(gas/aerosol variables: mass mixing ratios)

GAS-PHASE CHEM (52 species) → *Jorba et al. (JGR 2012)* → *Badia and Jorba (AE 2014)*

DUST (8 bins) → *Pérez et al. (ACP 2011)* → *Haustein et al. (ACP 2012)*

SEA-SALT (8 bins) → *Spada et al. (ACP 2013)*

BC/OM/SO4 → *under dev.*



METEOROLOGY CHEMISTRY ON-LINE INTERACTIONS TAKEN INTO CONSIDERATION BY NMMB/BSC-CTM MODEL AND ITS FUTURE DEVELOPMENTS

$$\partial_t Q_{i,j} + (\vec{v}\cdot\vec{\nabla}) Q_{i,j} = \sum_k \frac{dQ_{i,j}}{dt}(u^*, \vec{q}_w, \vec{c}_g, \ldots)\Big|_{aero,k}$$

$$\partial_t \rho_{d,a} + \vec{\nabla}(\rho_{d,a}\vec{v}) = 0$$

$$\partial_t \vec{v} + (\vec{v}\cdot\vec{\nabla})\vec{v} = -f\vec{k}\times\vec{v} - \vec{\nabla}\Phi - \frac{1}{\rho_a}\vec{\nabla}p + \frac{d\vec{v}}{dt}\Big|_{turb}$$

$$\partial_t T + (\vec{v}\cdot\vec{\nabla}) T = \sum_k \frac{dT}{dt}(I_\lambda, \ldots)\Big|_{diab,k} + \frac{dT}{dt}\Big|_{turb}$$

$$\partial_t q_{w,\eta} + (\vec{v}\cdot\vec{\nabla}) q_{w,\eta} = \sum_k \frac{dq_{w,\eta}}{dt}\Big|_{water,k}$$

$$p\alpha = RT$$

$$\partial_t c_{g,\gamma} + (\vec{v}\cdot\vec{\nabla}) c_{g,\gamma} = \frac{dc_{g,\gamma}}{dt}(\vec{c}_g, I_\lambda, \ldots)\Big|_{photochem,k} + \ldots$$

$$\frac{dI_\lambda}{dt} = f(I_\lambda, \tau_\lambda^{aero}, \omega_\lambda^{aero}, g_\lambda^{aero}, \ldots)$$

Radiative Transfer Eq.

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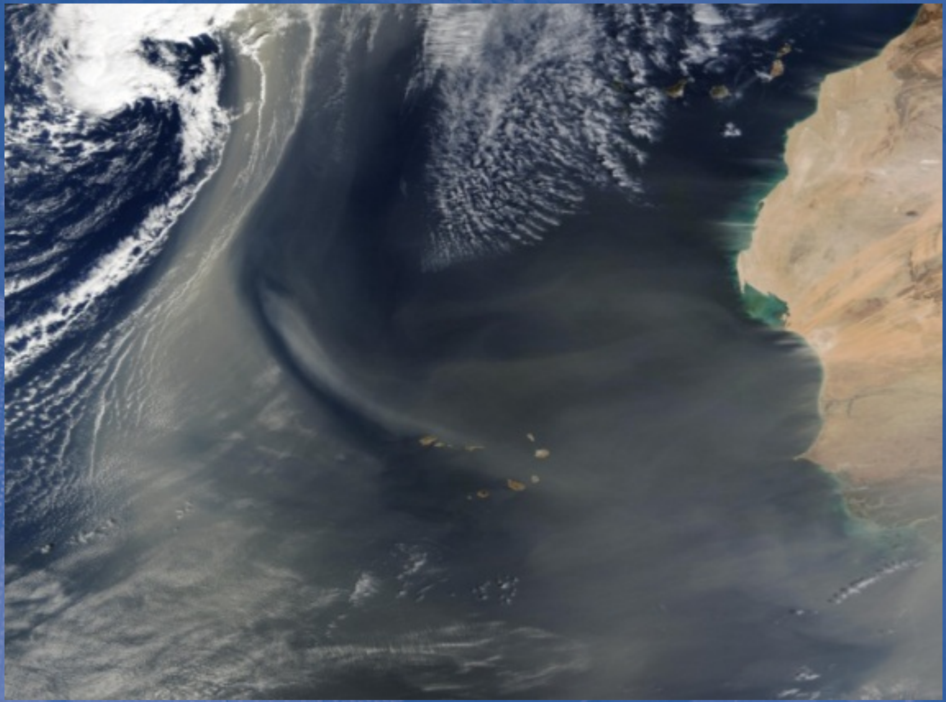


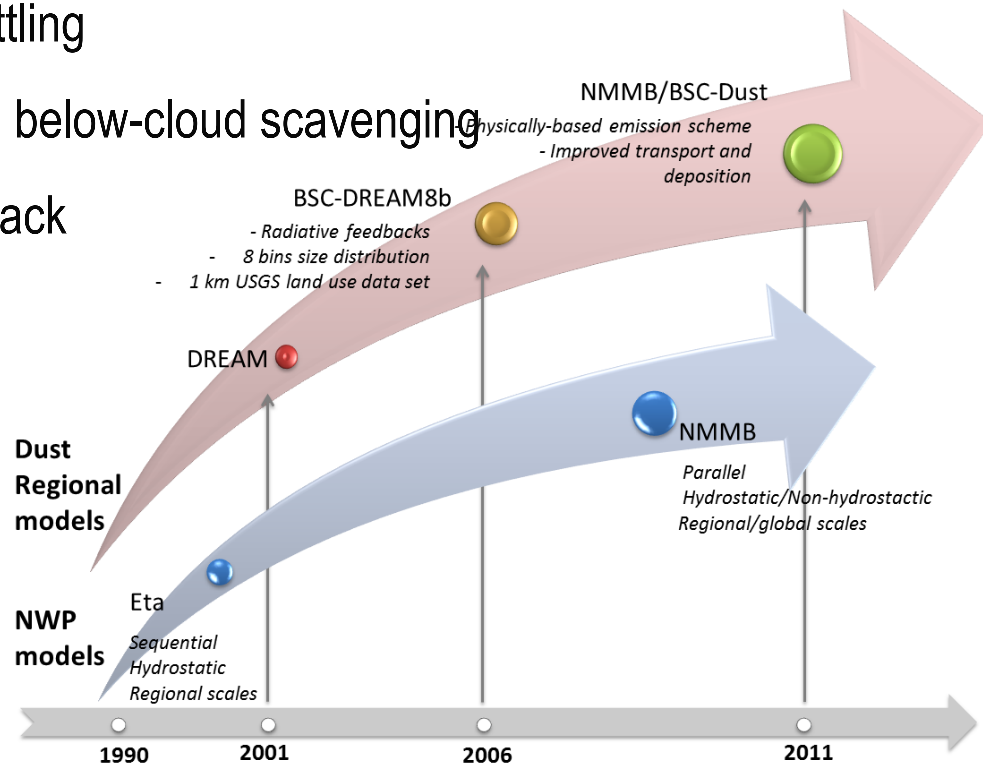
MINERAL DUST MODULE
DUST AOD DATA ASSIMILATION

NMMB/BSC-Dust model (Pérez et al., 2011)

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

Evolution from
Nickovic et al. (2001)
Pérez et al. (2006ab)



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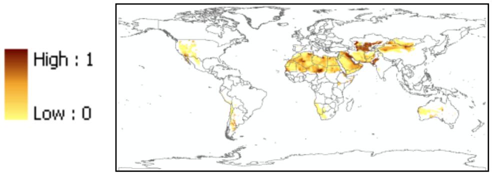
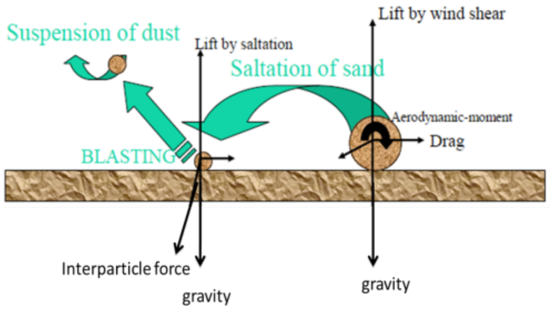
EMISSION SCHEME

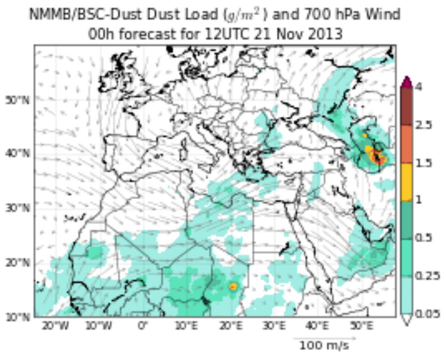


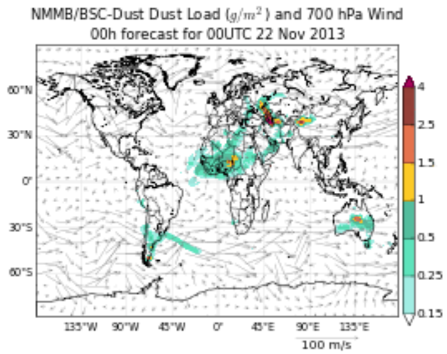
$\delta = USGS \cdot PREF \cdot (1 - VEGFRAC) \cdot (1 - SnowCover)$

- Source function: includes update land databases (vegetation fraction, land textures, soil types and albedo) and a preferential "topographic" source mask
- Physically-based emission scheme which includes saltation and sandblasting



DAILY DUST FORECAST AT BSC

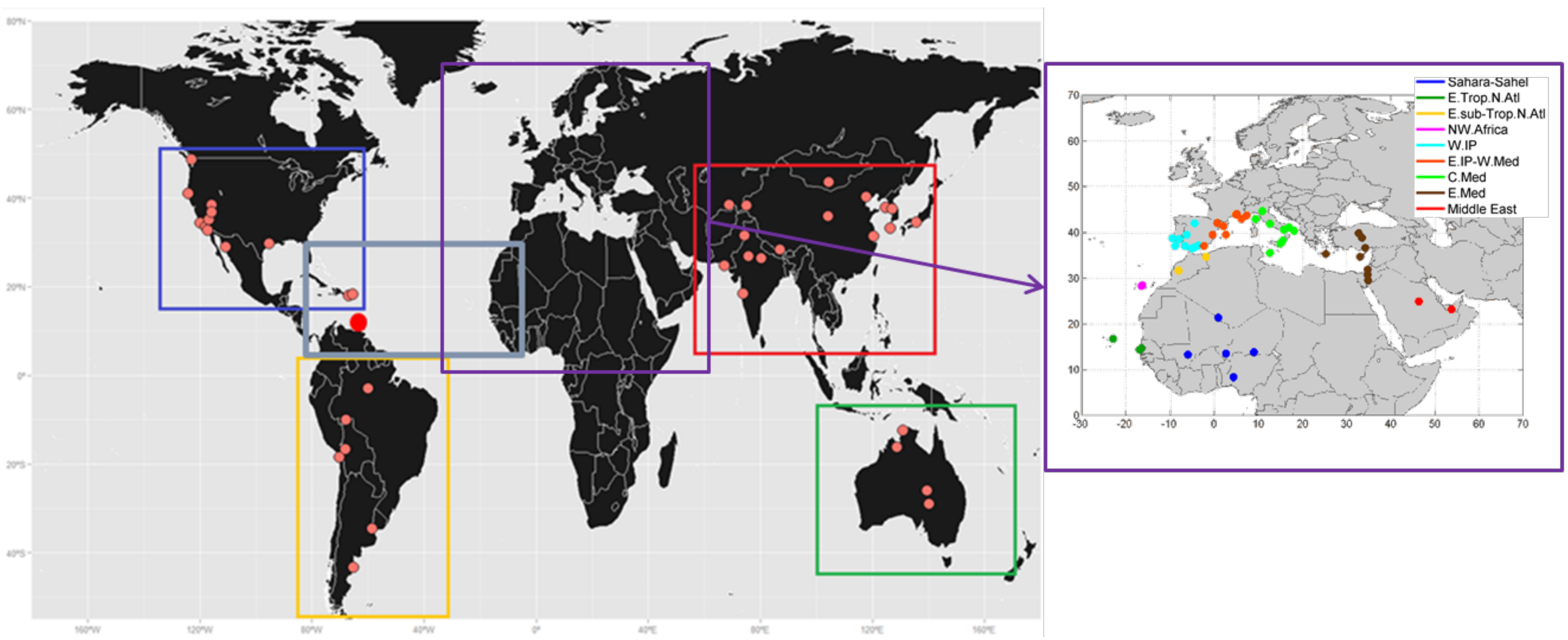




http://www.bsc.es/earth-sciences/mineral-dust/nmmbbsc-dust-forecast/

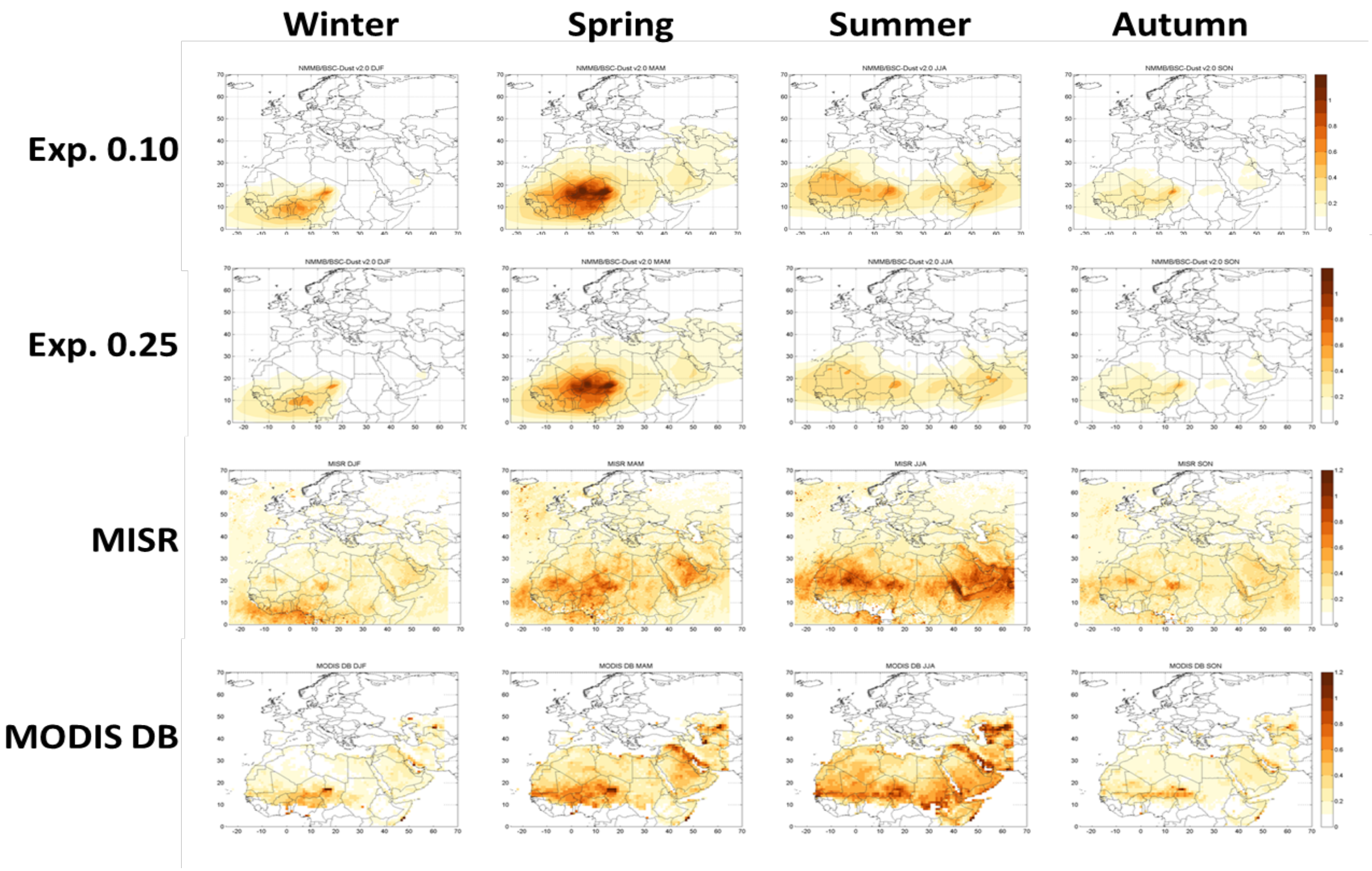
Evaluation methods

- Column-integrated AOD at 550 nm from AERONET Level 2.0
- Spectral Deconvolution Algorithm providing AODfine and AODcoarse
- Filter applied to the AERONET observations
  - AE<0.75 is considered in the calculations
  - AE>=0.75 not dust contribution, not considered for calculations
- RMSE, MB, correlation



- Satellite retrievals: MODIS, OMI, MISR, MSG

Dust AOD (550nm) year 2011



Qualitative Satellite intercomparison at different resolutions

	Exp. 0.10				Exp. 0.25				Exp. Glob.				Exp. Glob. Corrected			
Regions	*NDATA*	*r*	*RMSE*	*MB*	*NDATA*	*r*	*RMSE*	*MB*	*NDATA*	*r*	*RMSE*	*MB*	*NDATA*	*r*	*RMSE*	*MB*
Sahara-Sahel	3266	0,54	0,38	-0,02	3337	0,56	0,36	-0,05	3337	0,52	1,54	1,00	3337	0,52	0,41	-0,02
E.Trop.N.Atl	2177	0,68	0,27	-0,17	2218	0,70	0,26	-0,17	2218	0,47	0,78	0,56	2218	0,47	0,30	-0,14
E.sub-Trop.N.Atl	1237	0,69	0,19	-0,12	1274	0,72	0,19	-0,12	1274	0,69	0,23	0,06	1274	0,69	0,21	-0,13
NW. Africa	2209	0,77	0,10	-0,06	2254	0,76	0,10	-0,05	2254	0,72	0,18	0,08	2254	0,72	0,11	-0,05
W.IP	4805	0,73	0,09	-0,03	4941	0,76	0,09	-0,03	4941	0,69	0,15	0,07	4941	0,69	0,10	-0,02
E.IP-W.Med	4821	0,67	0,07	-0,01	4971	0,69	0,07	-0,01	4971	0,64	0,15	0,08	4971	0,64	0,07	0,01
C. Med	5453	0,66	0,09	-0,01	5595	0,67	0,08	-0,01	5595	0,56	0,22	0,11	5595	0,56	0,10	0,01
E. Med	4089	0,51	0,12	-0,01	4176	0,54	0,12	-0,01	4176	0,54	0,24	0,15	4176	0,54	0,12	0,00
West Asia	1238	0,34	0,45	-0,30	1240	0,37	0,43	-0,30	1240	0,37	0,47	0,29	1240	0,37	0,43	-0,31
NAMEE	***29295***	***0,73***	***0,20***	***-0,05***	***29446***	***0,75***	***0,19***	***-0,05***	***29446***	***0,70***	***0,54***	***0,25***	***29446***	***0,70***	***0,20***	***-0,03***

Quantitative evaluation against AERONET measurements

Data Assimilation for NMMB/BSC-CTM: Mineral Dust

- Enhancement of NMMB/BSC-CTM model with data assimilation using an ensemble technique: the **Local Ensemble Transform Kalman Filter** (LETKF)
  - it is particularly suited to high-performance computing applications: it allows a parallel computation of the analysis;
  - it uses flow-dependent background errors: the background error covariance is generated and propagated by the filter, using model dynamics;
  - it is easy to code: it does not require the development of adjoint code.

- Using a smoothed localisation of the observations:
  - observation influence decays gradually towards zero as their distance from analysis location increases.

- Testing the assimilation of NRL MODIS AOD:
  - a Level 3 filtered, corrected, and aggregated product, with a retrieval error also provided.

- The following preliminary tests are focused on mineral dust and on low resolution runs of our global model.

Vertical mass flux of dust into a transport bin *k*

$$F_k = C\, S\,(1 - V)\,\alpha\, H \sum_{i=0}^{3} m_i\, M_{i,k} \qquad k = 1, \cdots, 8$$

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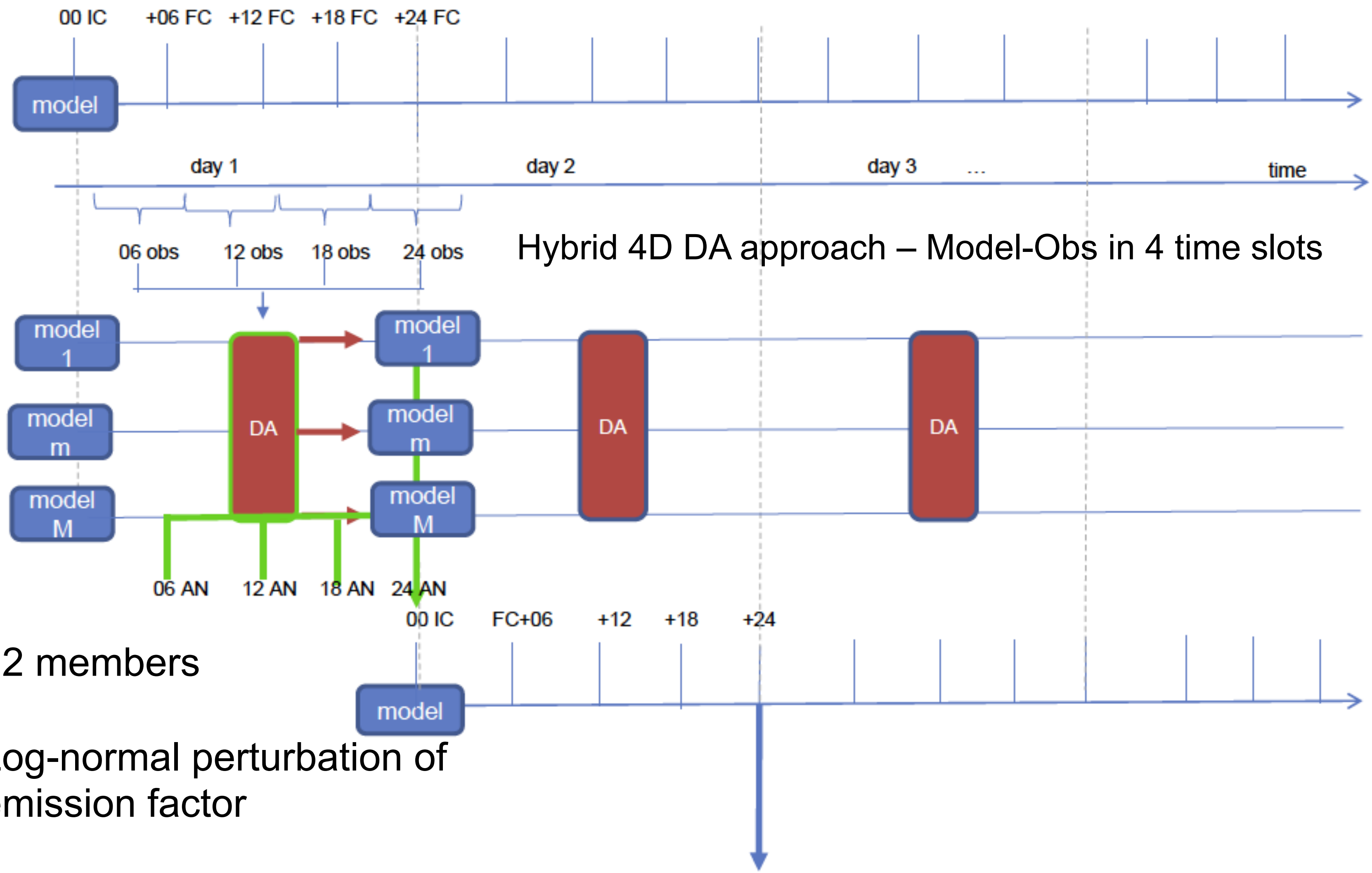
Data Assimilation Flow



Hybrid 4D DA approach – Model-Obs in 4 time slots

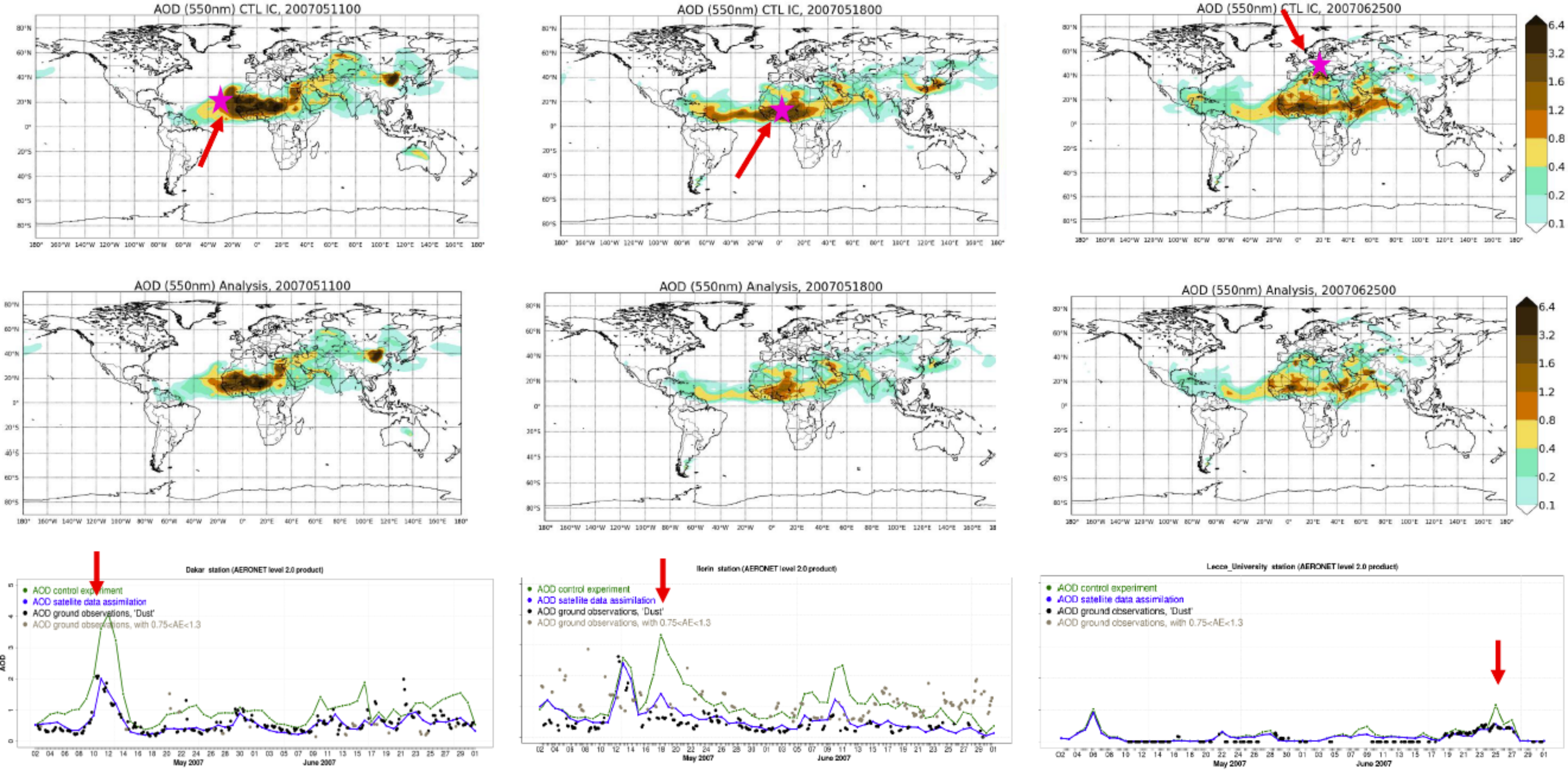
12 members

Log-normal perturbation of emission factor

Experiments use a spin-up of 1 month w/o DA

Validation against independent observations

Short-range transport | Near sources | Long-range transport



AERONET stations

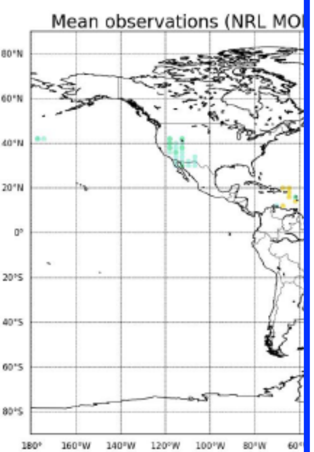
Black dot → dust AOD AE<=0.75 ;

Grey dots → uncertain type of AOD with 0.75<AE<1.3

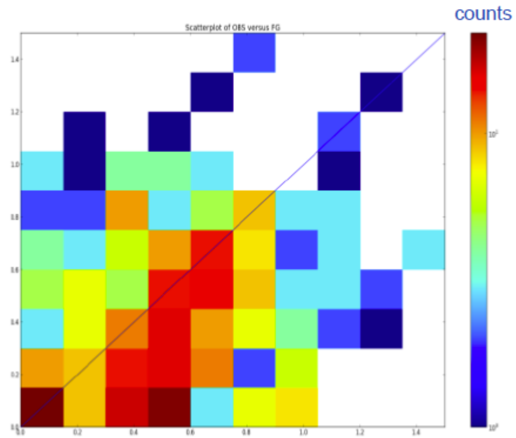
Quality control on the observations

6 hour NRL MODIS AOD are selected according to:

land:	sea:
AE<0.75 from daily MODIS Aqua or Terra products	if AOD>0.2, **FF<0.5** from 6 hour NRL MODIS
AND	if AOD<=0.2, **0.4<FF<0.5** from 6 hour NRL MODIS
AI>1.5 from daily OMI product	**AND**
	AI>1.5 from daily OMI product



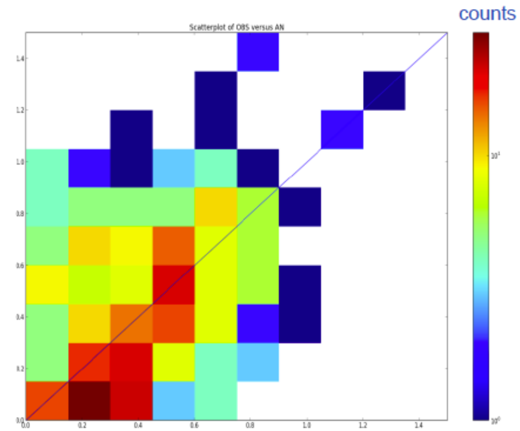
obs



first-guess

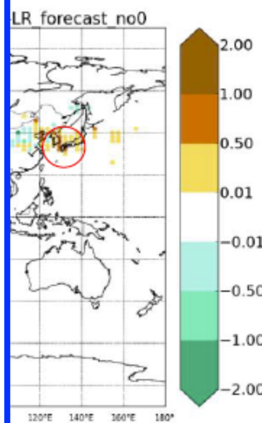
corr. coef. = 0.59

obs



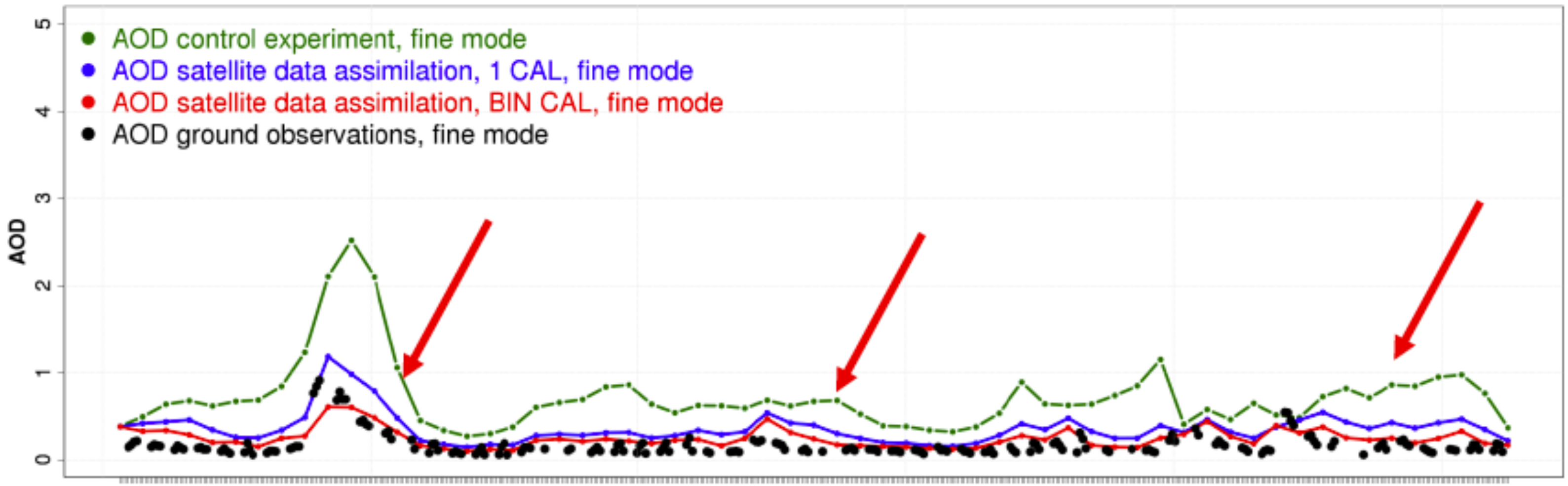
analysis

corr. coef. = 0.70

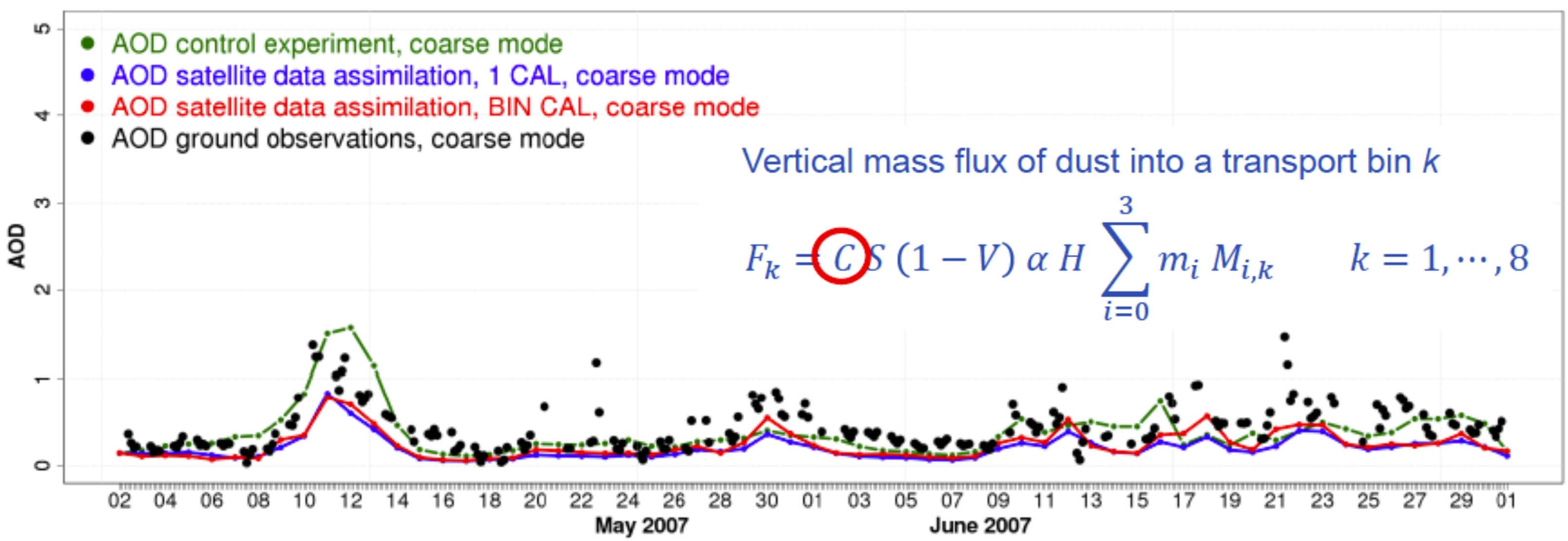


Impact of calibration factors per bin

Dakar station (AERONET SDA level 1.5 product)



Dakar station (AERONET SDA level 1.5 product)



Vertical mass flux of dust into a transport bin *k*

$$F_k = C\, S\,(1-V)\,\alpha\, H \sum_{i=0}^{3} m_i\, M_{i,k} \qquad k = 1,\cdots,8$$

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SEA SALT AEROSOL MODULE

SEA-SALT MODULE (Spada et al., 2013)

- ***assumptions:***

→ sea-salt (SS) externally mixed with dust (DU)

→ prognostic variables: 8 bins (dry mass mixing-ratios)

→ bins range from 0.1μm to 15μm 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

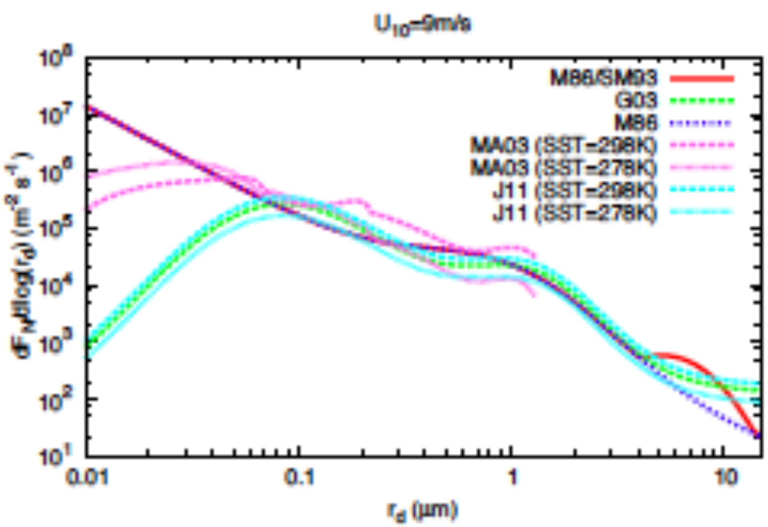
→ surf-zone production not considered in this work

SEA-SALT MODULE (emissions)

dF/dr = f(r, **ξ**)

M86 → ξ = U10 (bubbles)
G03 → ξ = U10 (bubbles, spume?)
M86/SM93 → ξ = U10, U_T=9m/s (bubbles, spume)
M86/SM93/MA03 → **ξ** = (U10, U_T, SST) (bubb., sp.)
J11 → **ξ** = (U10, SST) (bubb., sp.)

Monahan et al. (OW 1986)
Gong et al. (GBC 2003)
Smith et al. (RMS/QJ 1993)
Martensson et al. (JGR 2003)
Jaeglé et al. (ACP 2011)



criteria:
· whitecap method
· simplest (low number of parameters)
· bubbles and spume mechanisms

(M86, G03 and J11 extended up to 15μm)

→ **strong differences**
for r_d>5μm (spume)
and for 0.1μm<r_d<1μm (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)

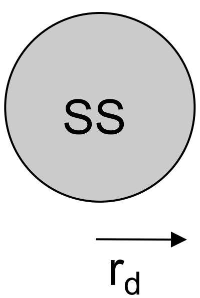
RH(%)	ϕ
< 50	1.0
50 – 70	1.6
70 – 80	1.8
80 – 90	2.0
90 – 95	2.4
95 – 99	2.9
> 99	4.8

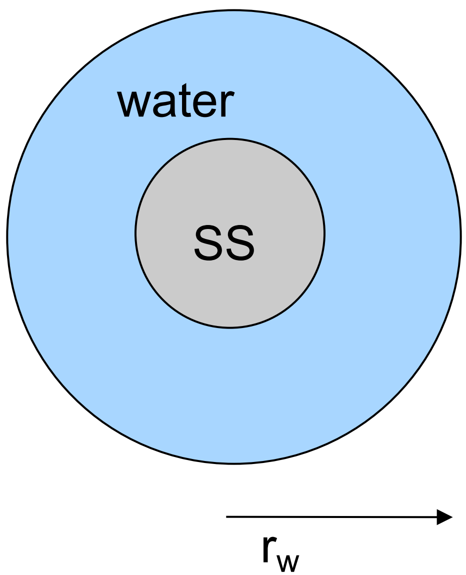
$$r_d \rightarrow r_w = r_d \cdot \Phi(RH)$$

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

(...)

DRY BINS:
· **hor. transport**
· **emissions**





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**

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SSA evaluation: sconc and AOD

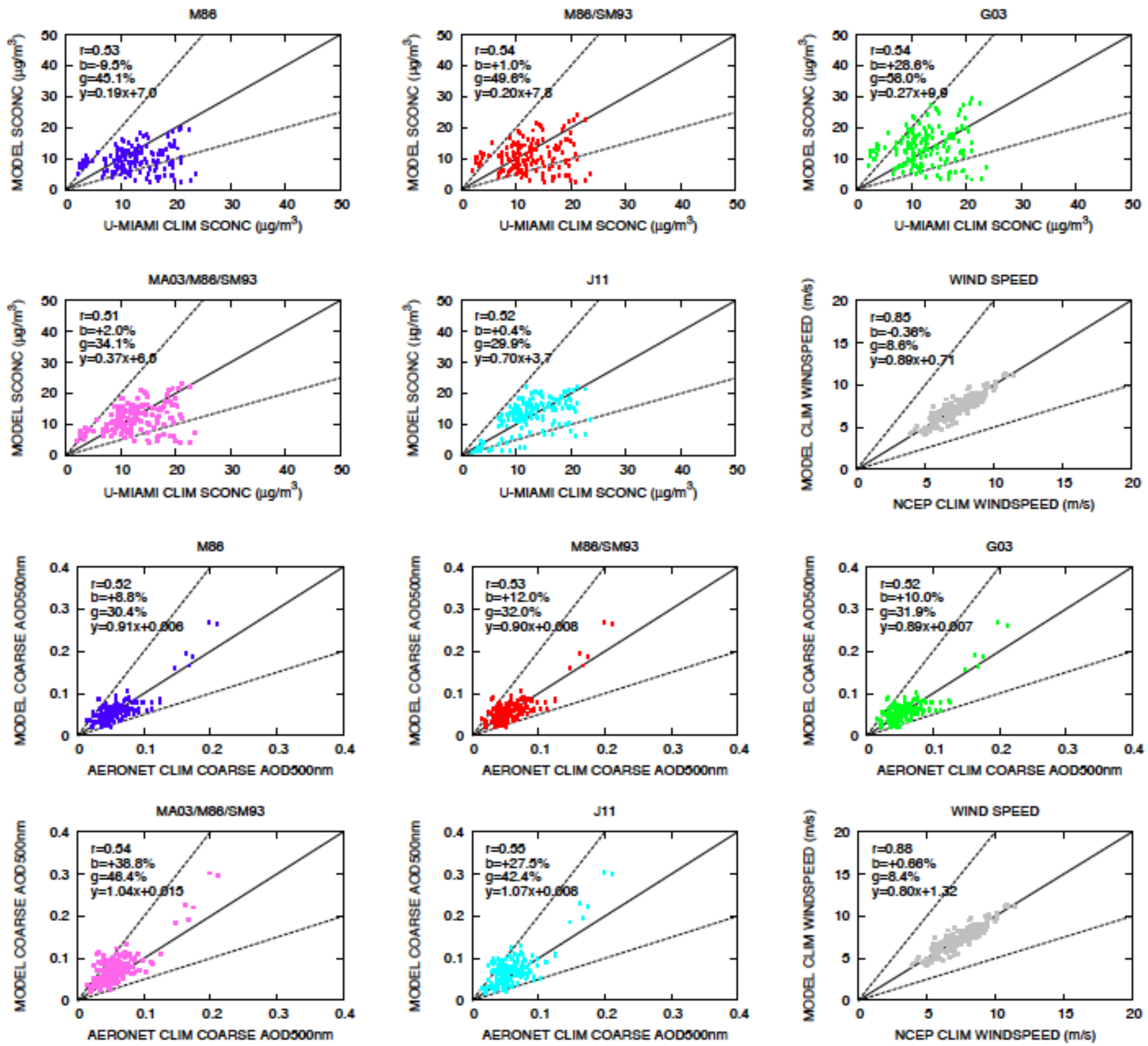
→ Surface monthly mean concentrations from U. Miami network

→ 2002-2006 runs with dust+ssa

Larger differences in sconc than AOD

→ Monthly mean AOD

→ Best agreement J11



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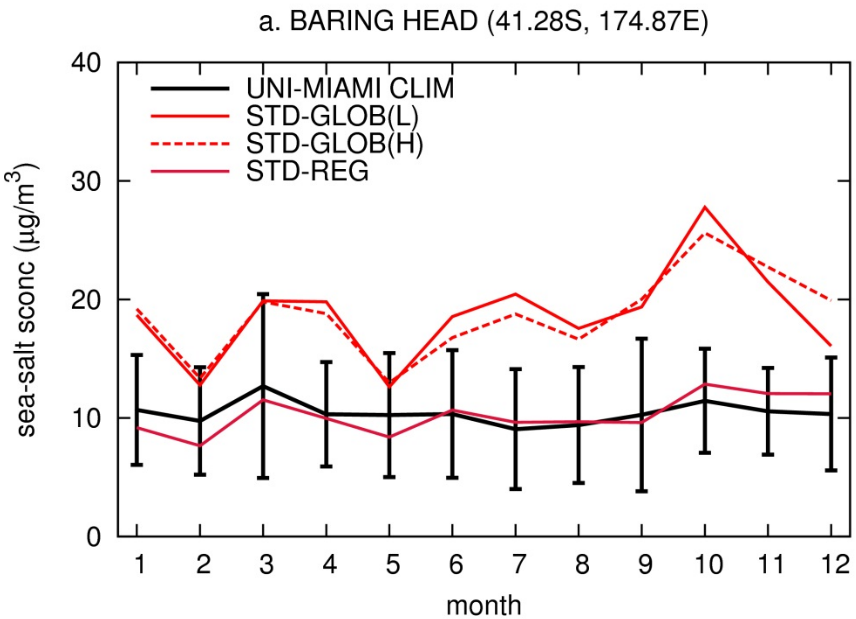
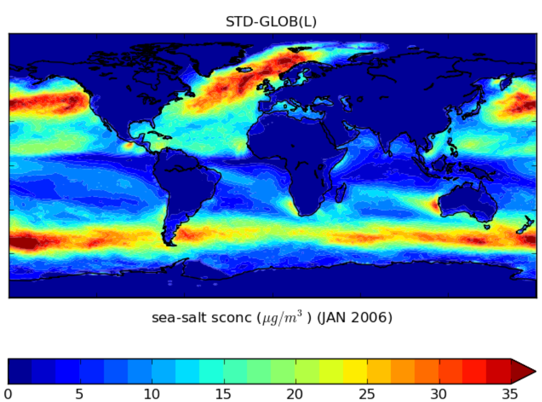
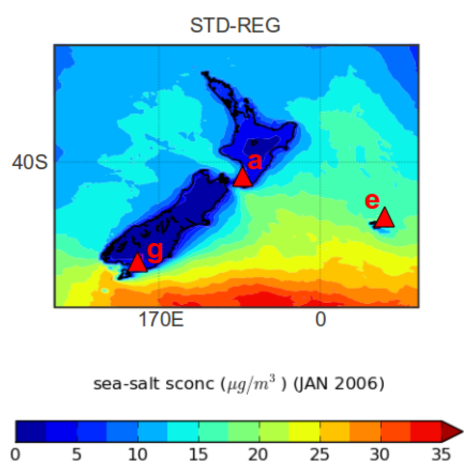
Impact of resolution

- 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 (≈0.1deg) effects may affect larger scales (>1deg)

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BC/OM/SULFATE MODULE

NMMB/BSC-CTM: Global Aerosols

previous version (until 2014):

- DUST (8 mass bins) ←Perez et al., 2011 (ACP)
- SEA-SALT (8 mass bins) ←Spada et al., 2013 (ACP)

new implementations (2014):

- BC (2 mass bins, phob/phil)
- POM (2 mass bins, phob/phil)
- SOA (4 mass bins → 2-product mechanism OR 1 bin → prescribed production, all phil)
- SO4 (1 mass bin, all phil)

related gases:

- SO2, DMS, H2O2, ISOP, TERP, ISOP-P1, ISOP-P2, TERP-P1, TERP-P2 (transported)
- OH, O3, HO2 (off-line climatologies from NMMB/BSC-CTM full gas-phase simulations)

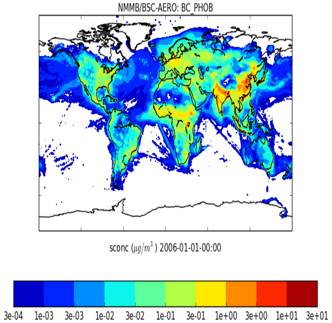
emissions:

- anthro: AEROCOM-ACCMIP emissions ←Lamarque et al., 2010 (ACP)
- DMS: AEROCOM EXP-I ← Dentener et al., 2006 (ACP)
- volcanic: AEROCOM-HC ← T. Diehl
- fires' injection height: under investigation...

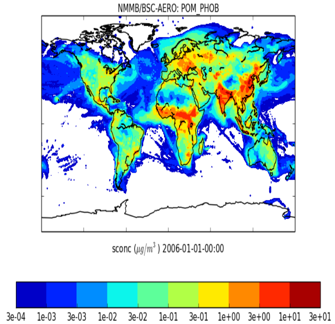
AOD calculation (we have a total AOD now):

- *GADS optical properties*
- *water-uptake depending on RH*

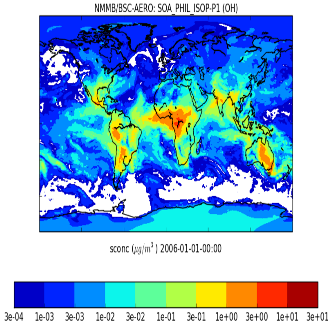
BC_PHOB



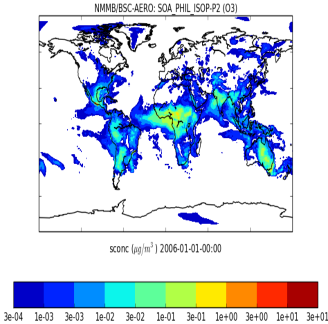
POM_PHOB



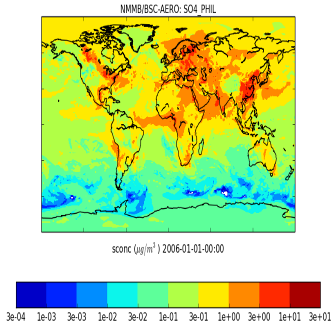
SOA_ISOP-P1



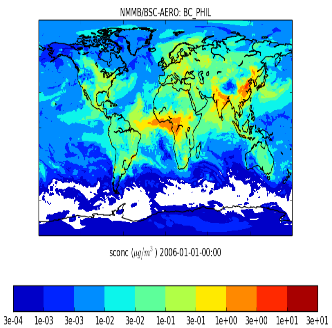
SOA_ISOP-P2



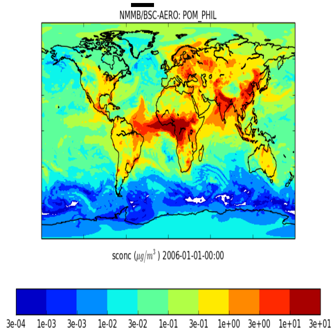
SO4_PHIL



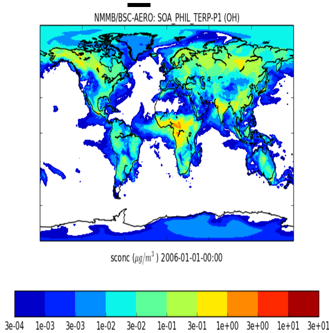
BC_PHIL



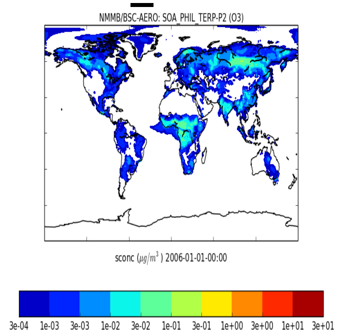
POM_PHIL



SOA_TERP-P1



SOA_TERP-P2



Surface conc. [μg/m^3]

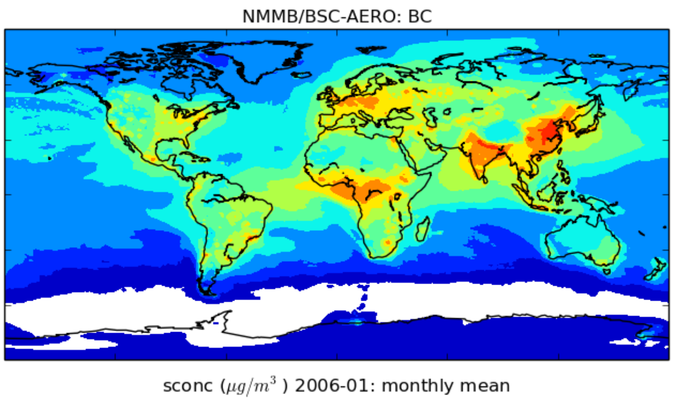
transported gases:				
-	-	ISOP-P1, TERP-P1	ISOP-P2, TERP-P2	SO2, DMS, H2O2
clim gases:				
-	-	OH	O3	OH, O3, HO2
emi phob/phil=0.8/0.2 phob-to-phil conv 1.2 days	emi phob/phil=0.5/0.5 OM/OC=1.6 phob-to-phil conv 1.2 days	MEGAN online emissions 2-products SOA mech ← Tsigaridis and Kanakidou, 2003 (ACP)		Sulfur chem (gas and aqueous phases) from MECCA mech (simplified) ← Sander et al., 2011 (GMD)

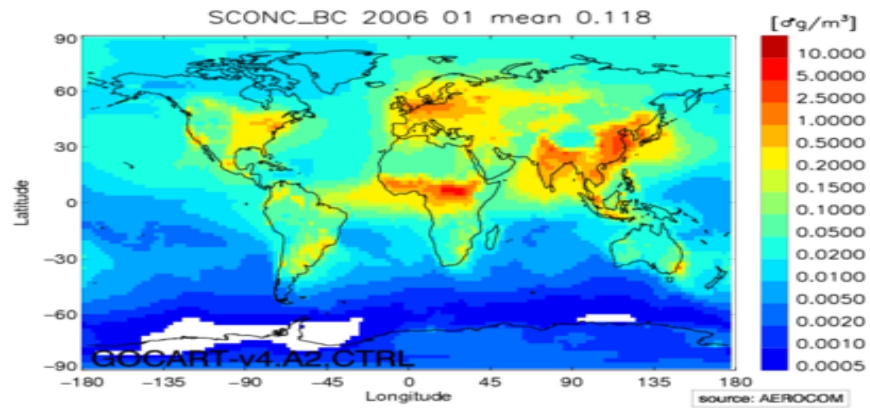
Preliminary RESULTS

JANUARY 2006 SCONC (monthly means)

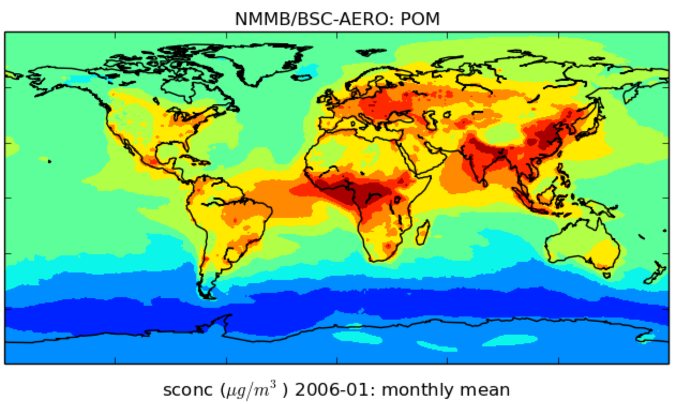
NMMB/BSC-CTM | **GOCART (AEROCOM EXP-II)**

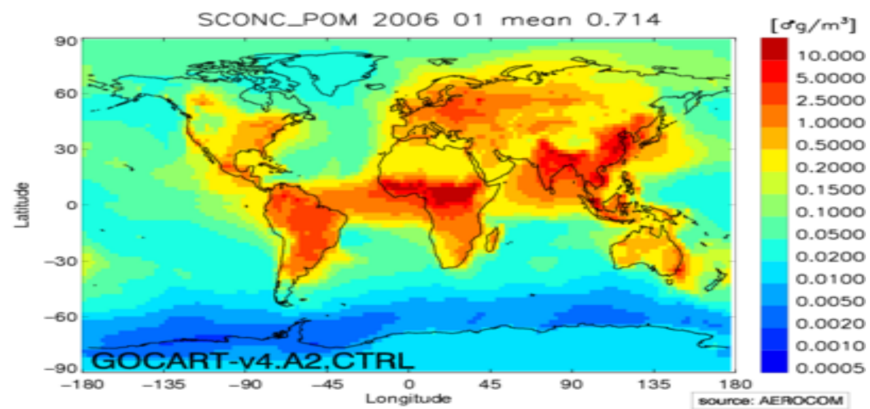
BC

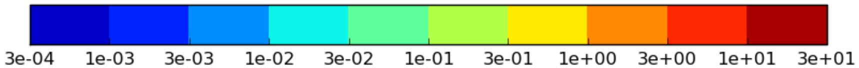




POM







Note: scales are not exactly the same

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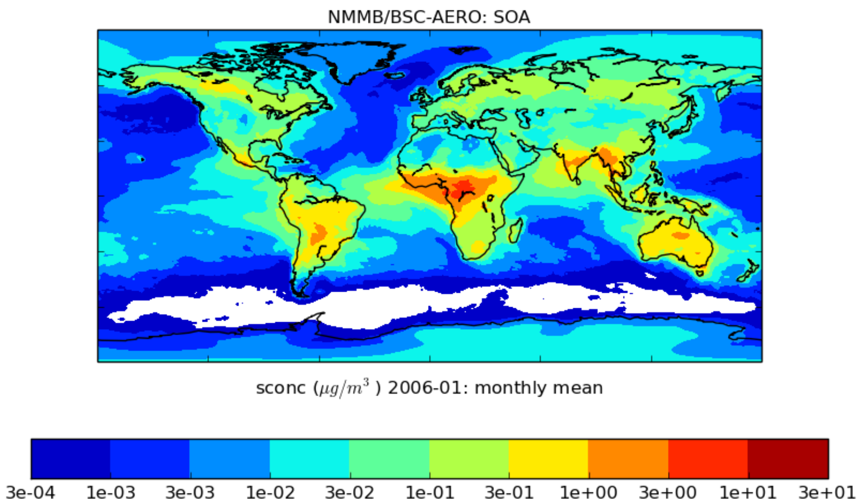
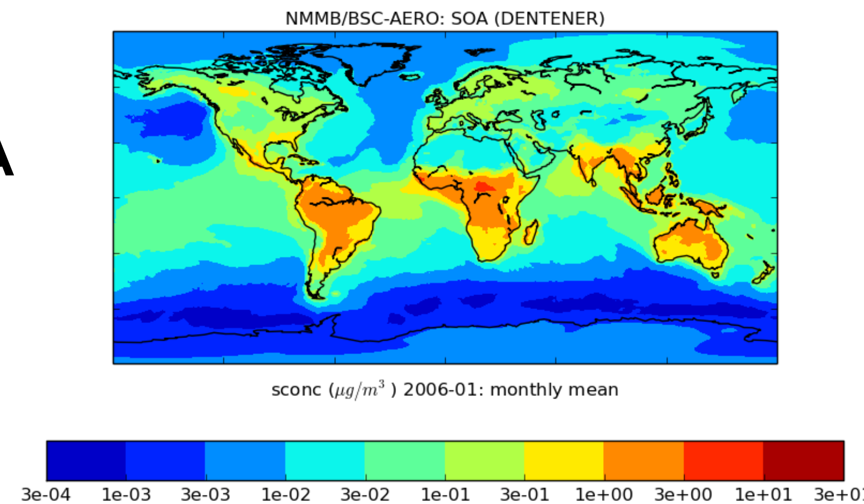
Preliminary RESULTS

JANUARY 2006 SCONC (monthly means)

NMMB/BSC-CTM (2-PRODUCTS SOA)

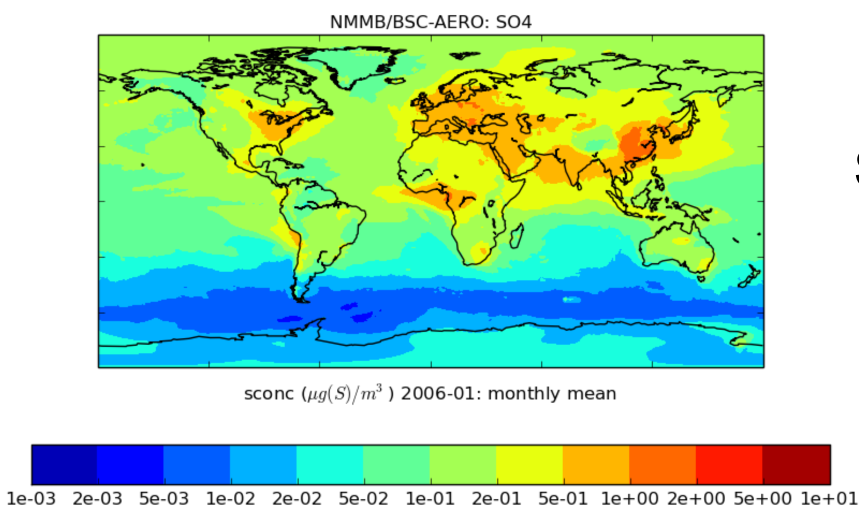


NMMB/BSC-CTM (DENTENER SOA)



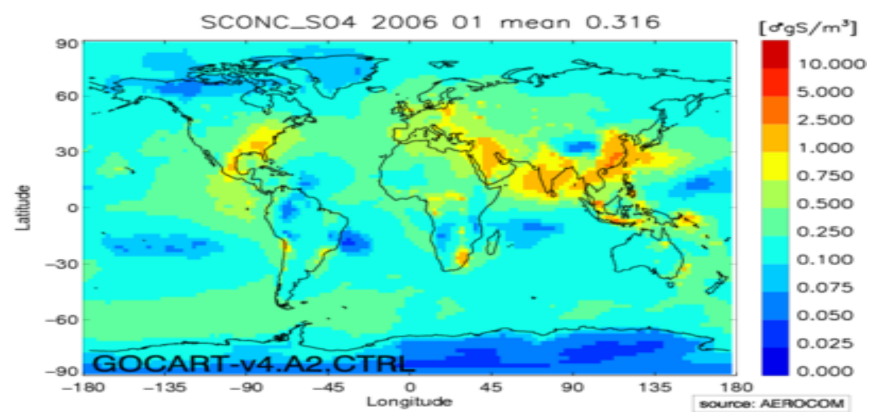
SOA

NMMB/BSC-CTM



SO4

GOCART (AEROCOM EXP-II)



Note: scales are not exactly the same

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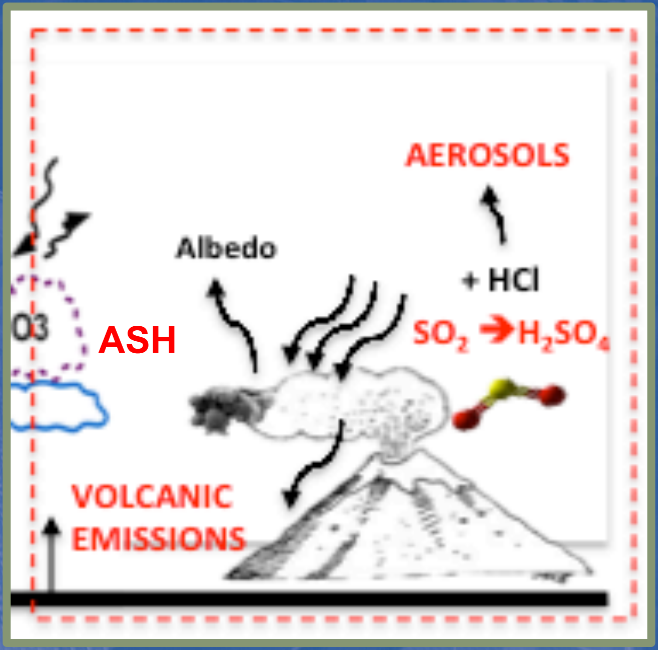
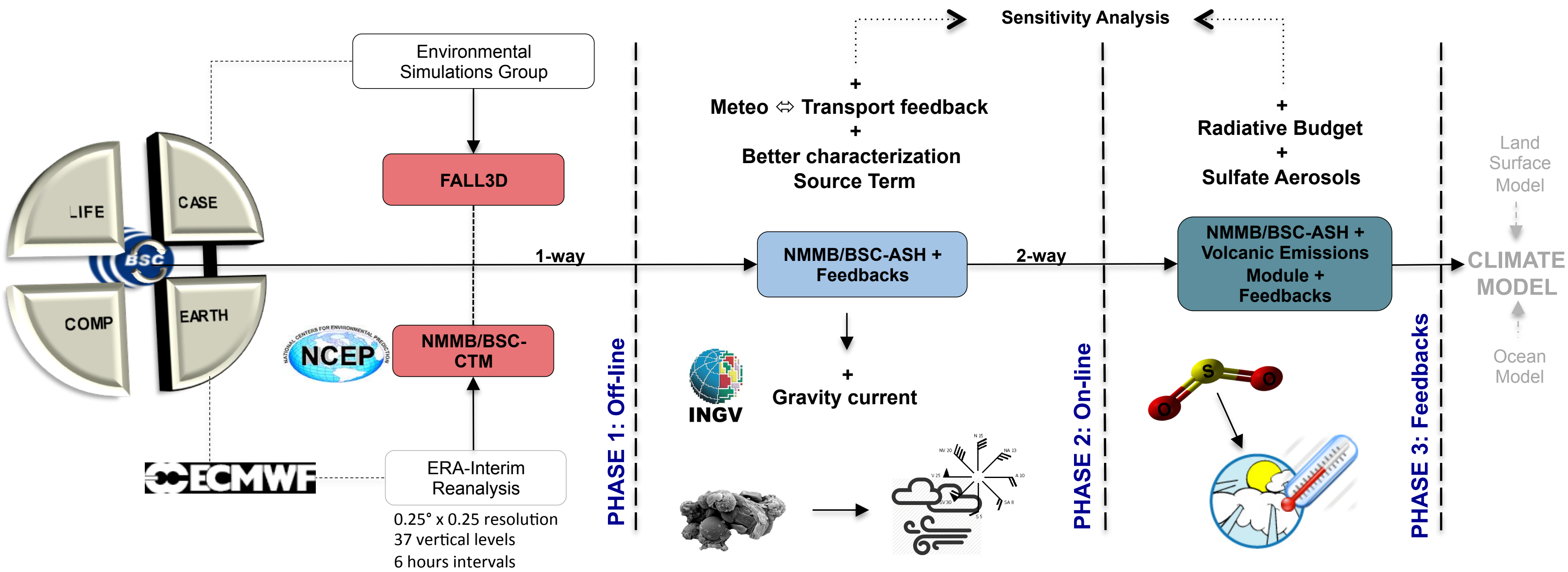


VOLCANIC ASH

Development Phases



2013 | 2014 | 2015

Phase 1 – Off-line validation

- Drive NMMB with Era-Interim data.
- Off-line simulations

Phase 2 – On-line coupling

- Implement a volcanic ash module .
- On-line coupling NMMB/BSC-ASH (*Martí et. al.* - in prep).
- Implement Gravity current effect (*Martí et. al.* - in prep).
- Off-line vs. On-line NMMB (*Martí et. al.* – working progress).
- Quantify feedbacks on meteorology (future).
- Improve source term.

Phase 3 - Two-way coupling and feedback

- Implement volcanic aerosol (SO_2) module.
- Couple the volcanic aerosol module with the existing NMMB/BSC-CTM radiative scheme.
- Quantify feedbacks on the radiative budget.

NMMB Off-line Simulations

Density driven transport in the umbrella region: Campanian Ignimbrite (CI) super-eruption (*Martí et. al.*, - in prep)

Motivation

Modelling distal dispersal of tephra fallout from ancient eruptions is very challenging:

- ~ 39 ka CI caldera-forming super-eruption is the largest volcanic eruption in Europe in the last 200 kyrs.
- Injected 250-300 km^3 of ash deposited over ~ 3.7 million km^2 implying significant climate and bio-cultural changes.

Problem

- Current models assume constant winds which is inadequate for ash dispersal in distal regions.
- Very challenging eruption to simulate since there is no meteorological winds on record for this eruption; 130 measured deposits available.
- No available VADT model to simulate ash dispersal on-line.

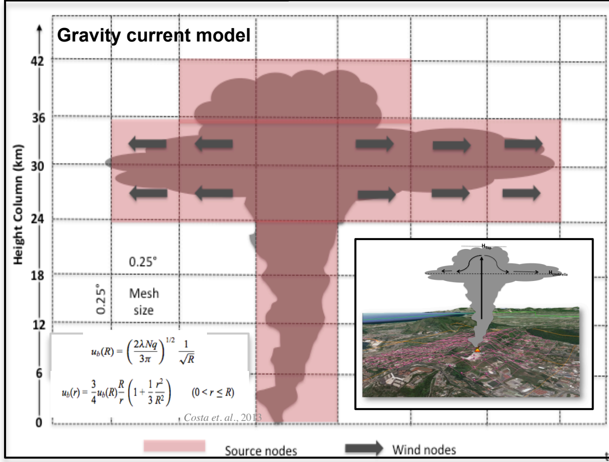
Methodology

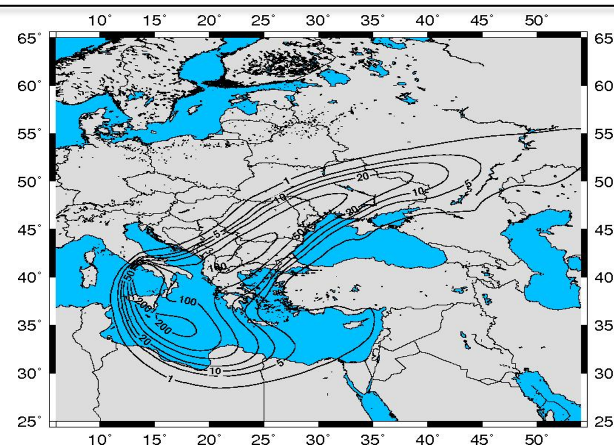
- Selection of the ERA-Interim meteorology fields that statistically represents best those at the time of the eruption.

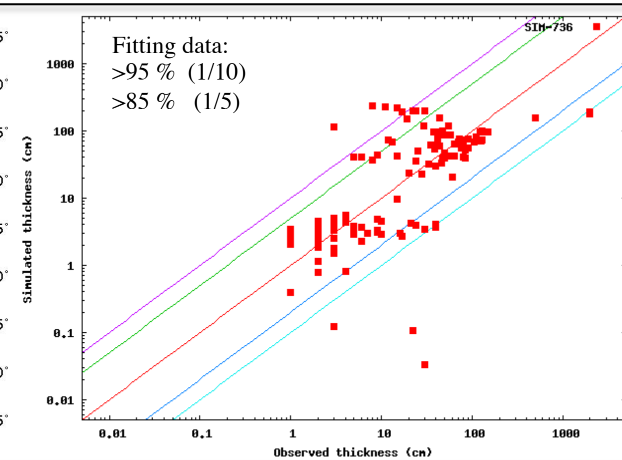
500 hundred synoptic meteorological ERA-40 fields (10 years) → Dispersal of particles (60μm & 1700kg/m³) → **300** wind fields potentially compatible with tephra dispersal observed → FALL3D: That best minimize the deviation of the regression for volcanological input param. → **10** wind field (0.5°x0.5°x2km) Mesh 121x101x25 → FALL3D: Mesh refinement around optimal values → **CI-173R and CI-330** (0.25°x0.25°x1km) Mesh 241x101x50 From *Costa et al., 2012*

- Implementation of a gravity current model under the NMMB/BSC-ASH.
- Off-line NMMB runs to reproduce ash dispersal and deposition for the CI super eruption.

Results







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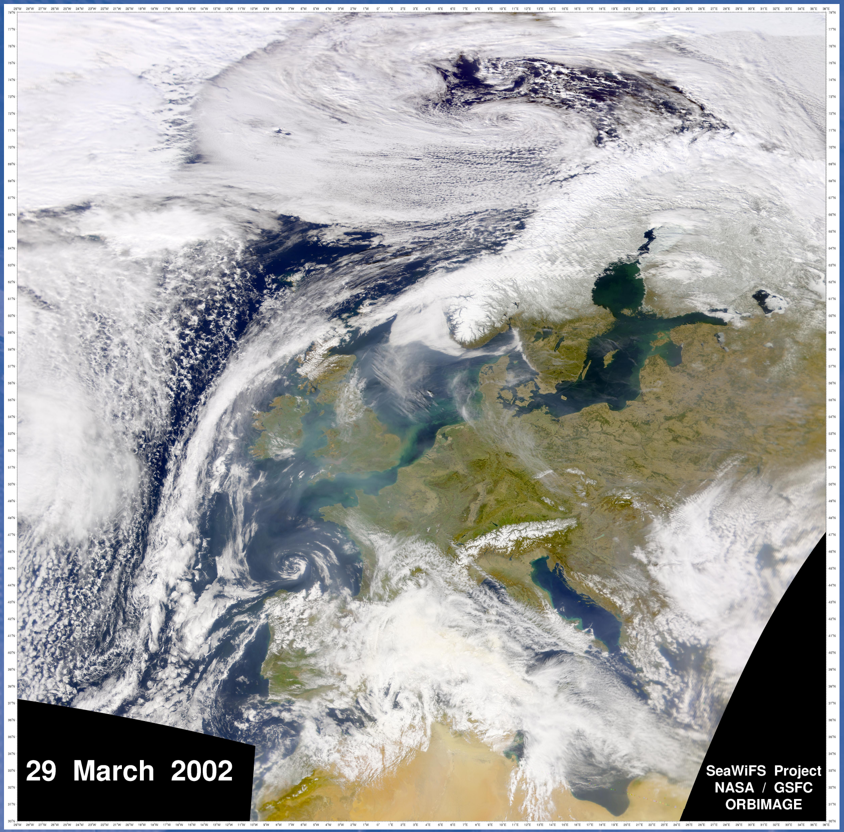


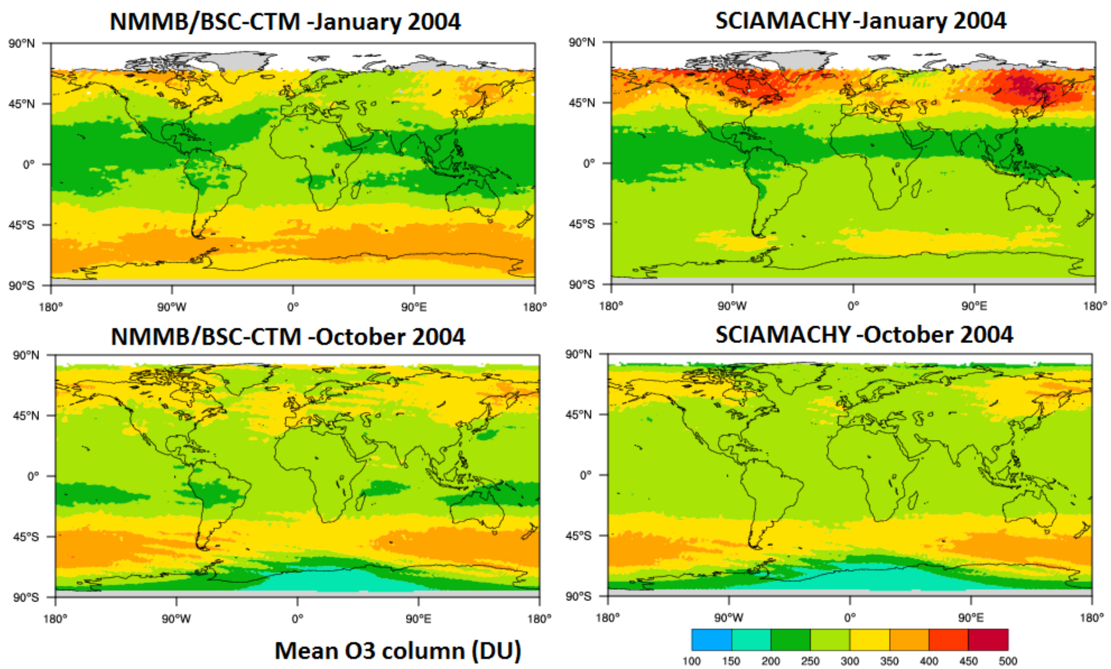
GAS-PHASE MODULE

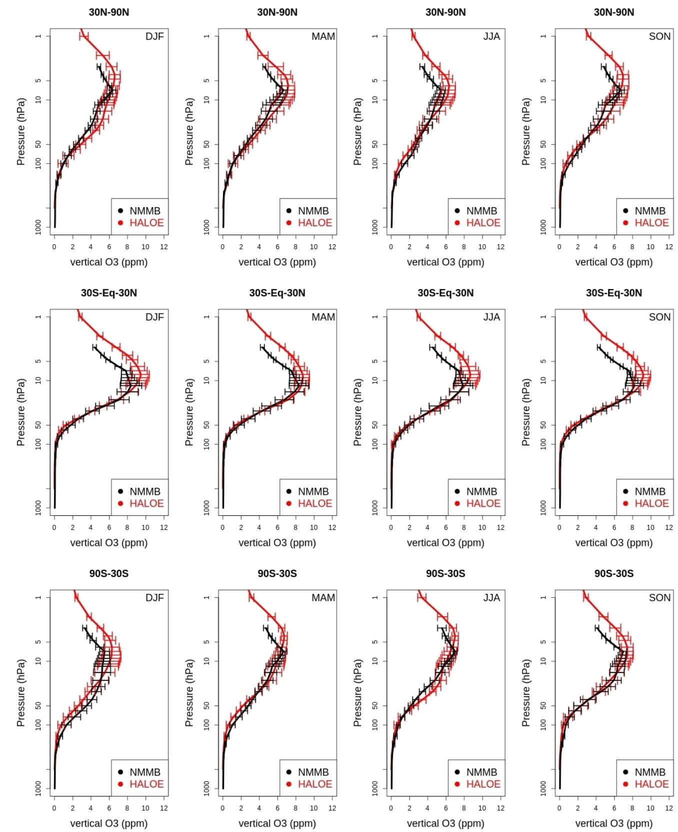
Model setup

→ Global domain
→ Non-hydrostatic physics
→ 1.4º x 1º horizontal resolution
→ 64 vertical (sigma-hybrid) layers
→ 1º x 1º NCEP/FNL analysis for meteorological initial conditions
→ Chemistry initial conditions from MOZART
→ Anthr. and BB emissions: ACCMIP
→ Biogenic emissions: MEGAN model
→ No lightning emissions
→ 1 year year spin-up
→ 2004 simulation

Meteorology	NMMB (Janjic and Gall, 2012)
Chemical Mechanism	CB05 (Yarwood et al., 2005)
Photolysis scheme	Fast-J (Wild et al., 2010)
Aerosols	Dust + SSA (Pérez et al., 2011; Spada et al., 2013) No secondary aerosols
Dry deposition	Wesely et al. (1986) gas, Pérez et al. (2011) aerosols
Wet deposition	Foley et al. (2010) gas, Zhang et al. (2001) aerosols
Direct effect	Mineral dust

Ozone atmospheric column (Badia et al., under preparation)





Satellite comparison: SCIAMACHY and HALOE

- COPCAT (Monge-Sanz et al., 2011) linear model for stratospheric ozone
- Coupled with the tropospheric mechanism of the CTM

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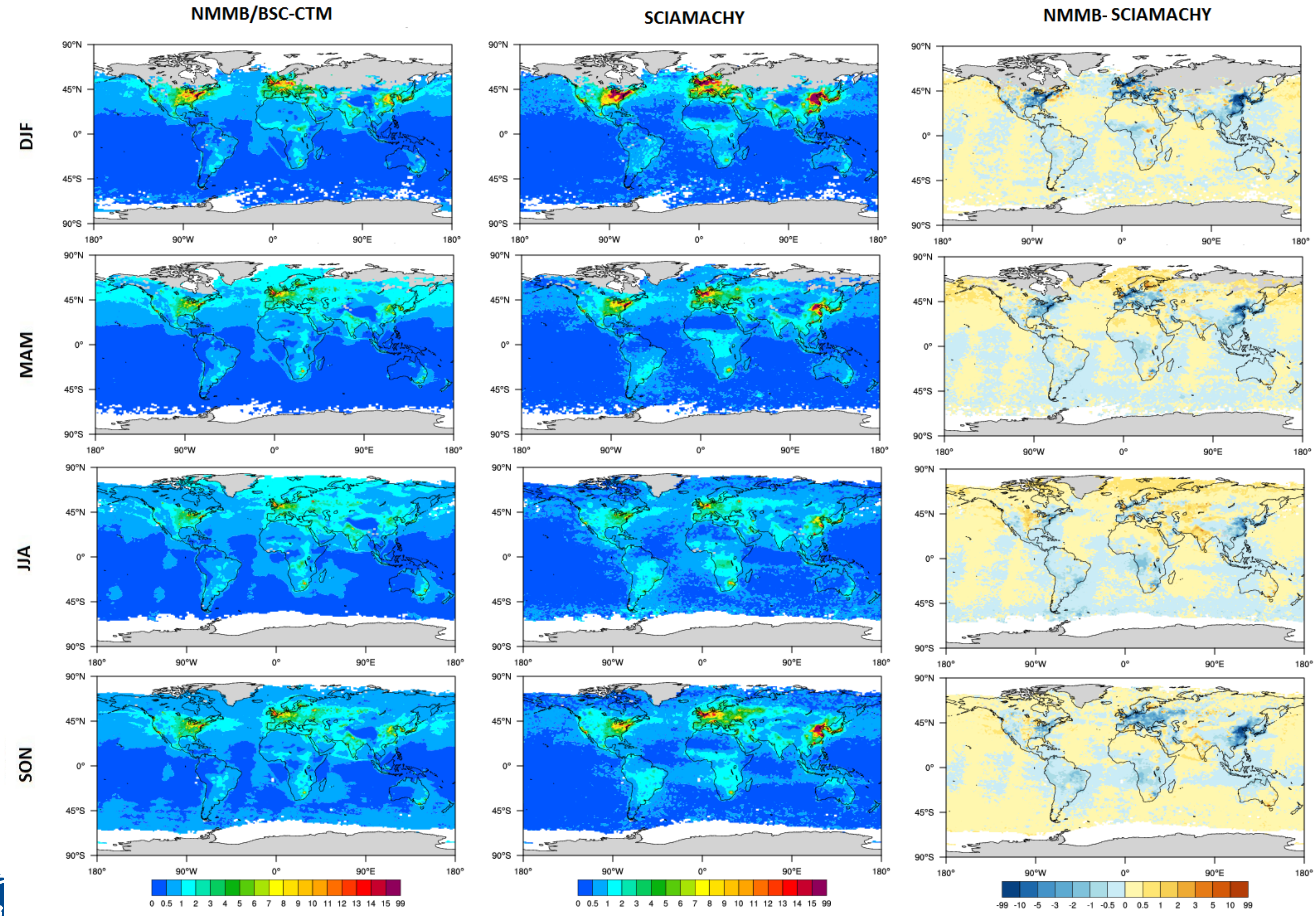
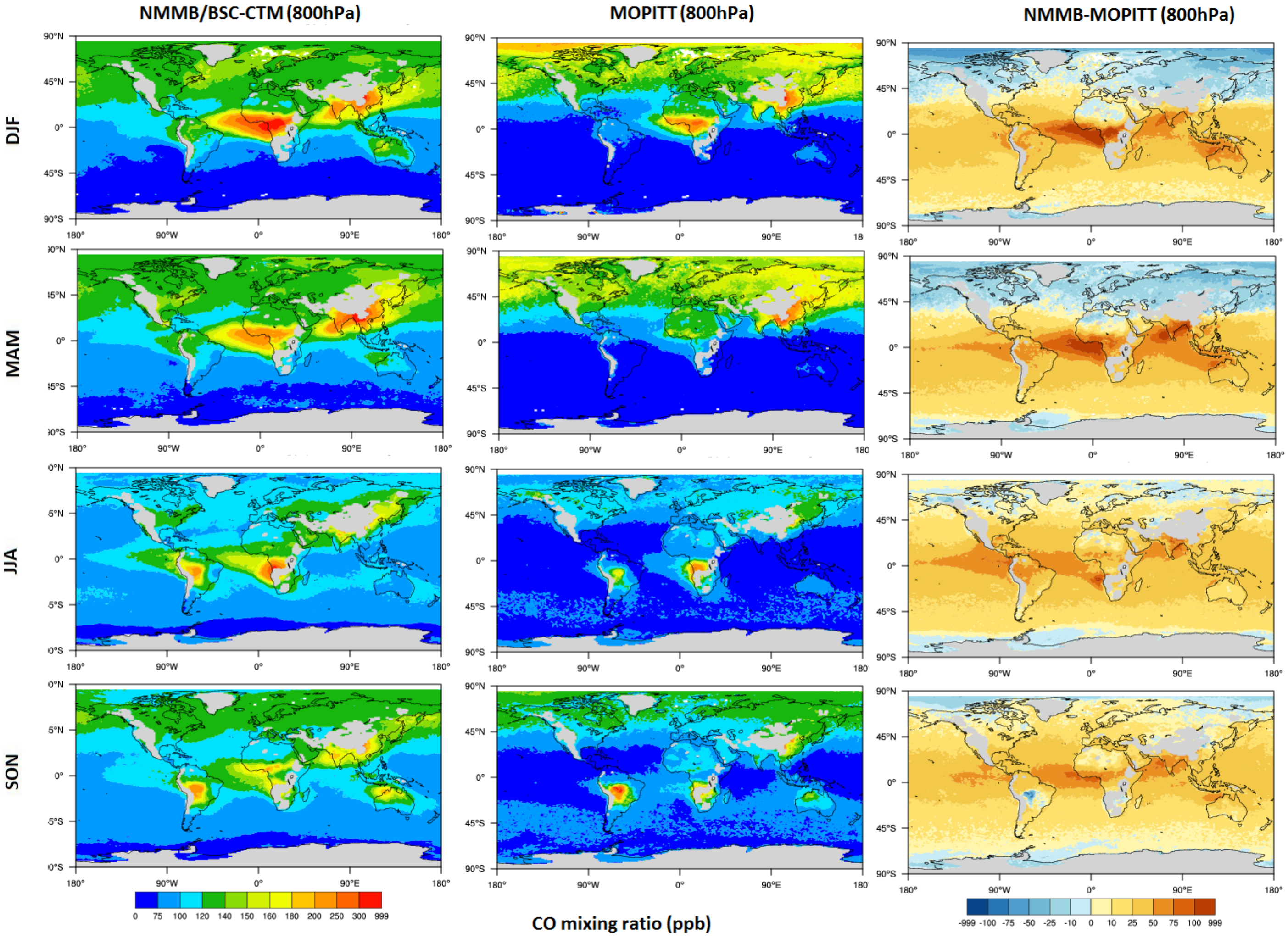
NO_2 Vertical Tropospheric Column



CO at 800 hPa: comparison with MOPITT (v5)



- Strong overestimations over fire regions.
- Good agreement over polluted areas.
- Need to implement attenuation of radiation due to aerosols in photolysis scheme.

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Regional Experiment configuration – AQMEII-Phase2

Period: Run one year simulation (2010).

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

Chemical BC: MACC (IFS-MOZART)

Meteorological BC: NCEP/FNL 1ºx1º

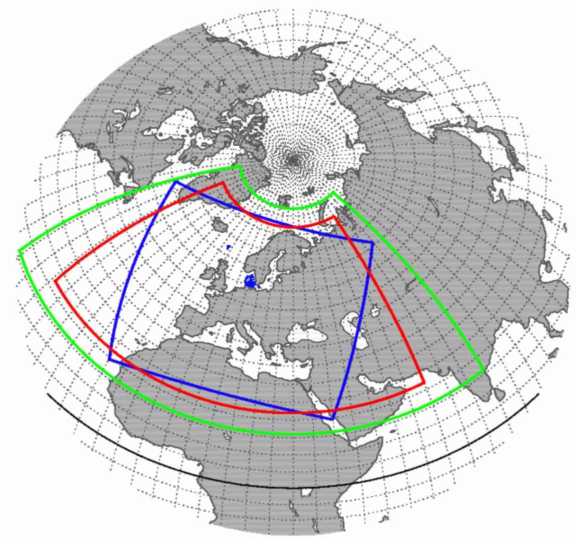
Emissions: TNO-MACC; Biogenics: MEGAN; No Fire Emissions

Horizontal Resolution: 0.2º x 0.2º

Vertical Resolution: 24 (and 48) top 50hPa

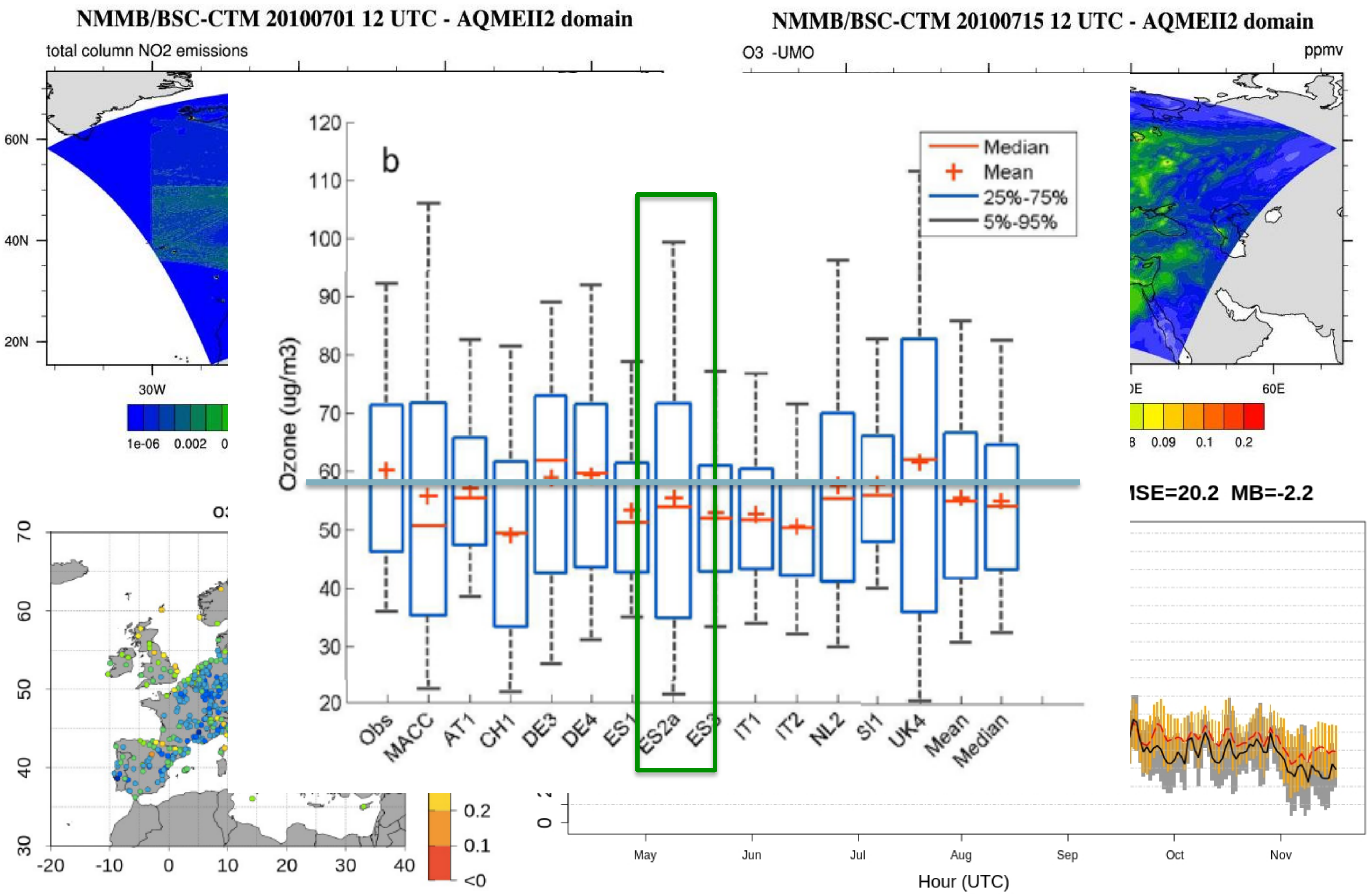
Gas Chemical mechanism: CB05

Aerosols: only dust-ssa

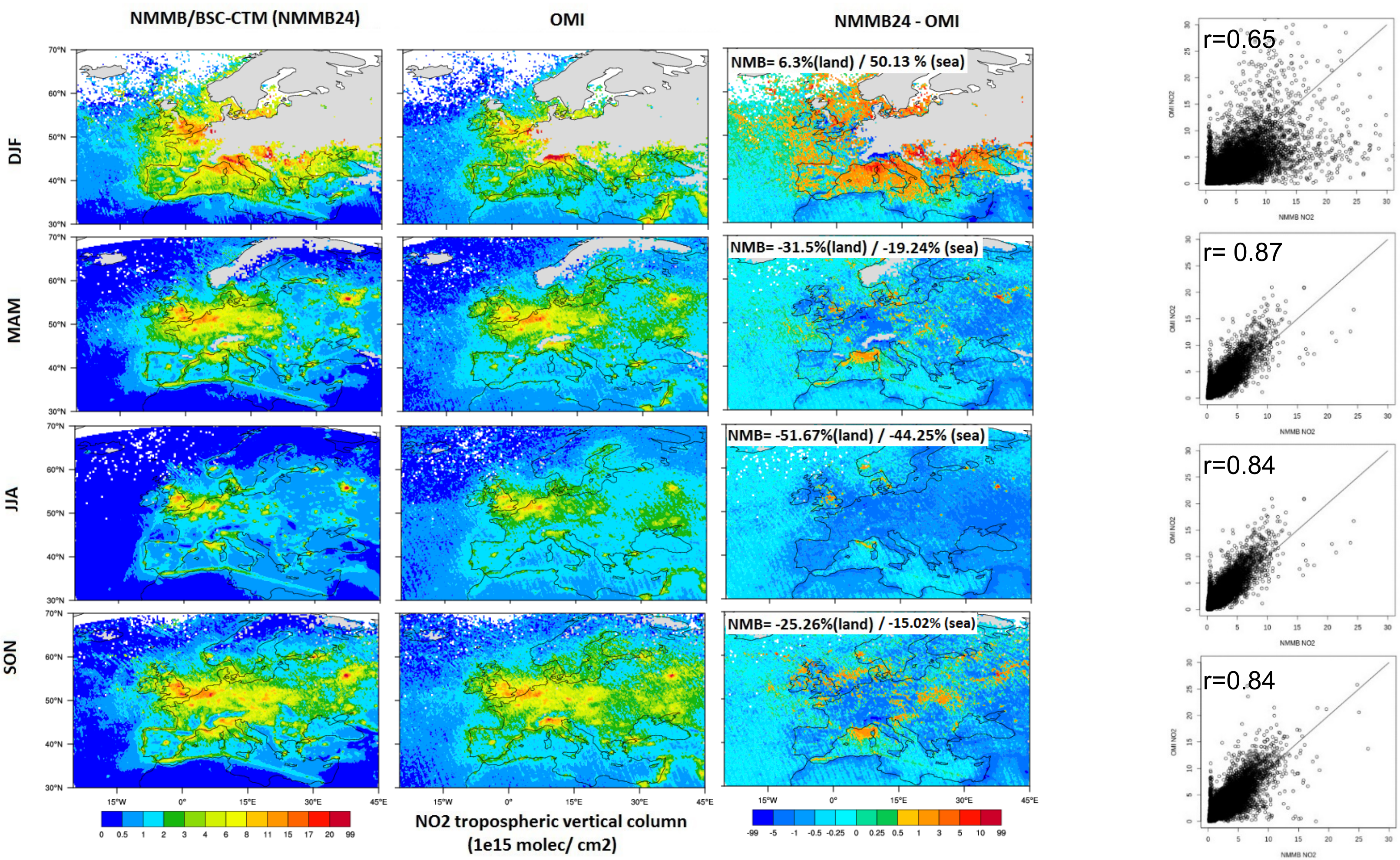


Blue: model domain
Red: AQMEII domain (to submit)
Green: BC domain

Regional run results (Badia and Jorba, 2014; Ulas et al., 2014)



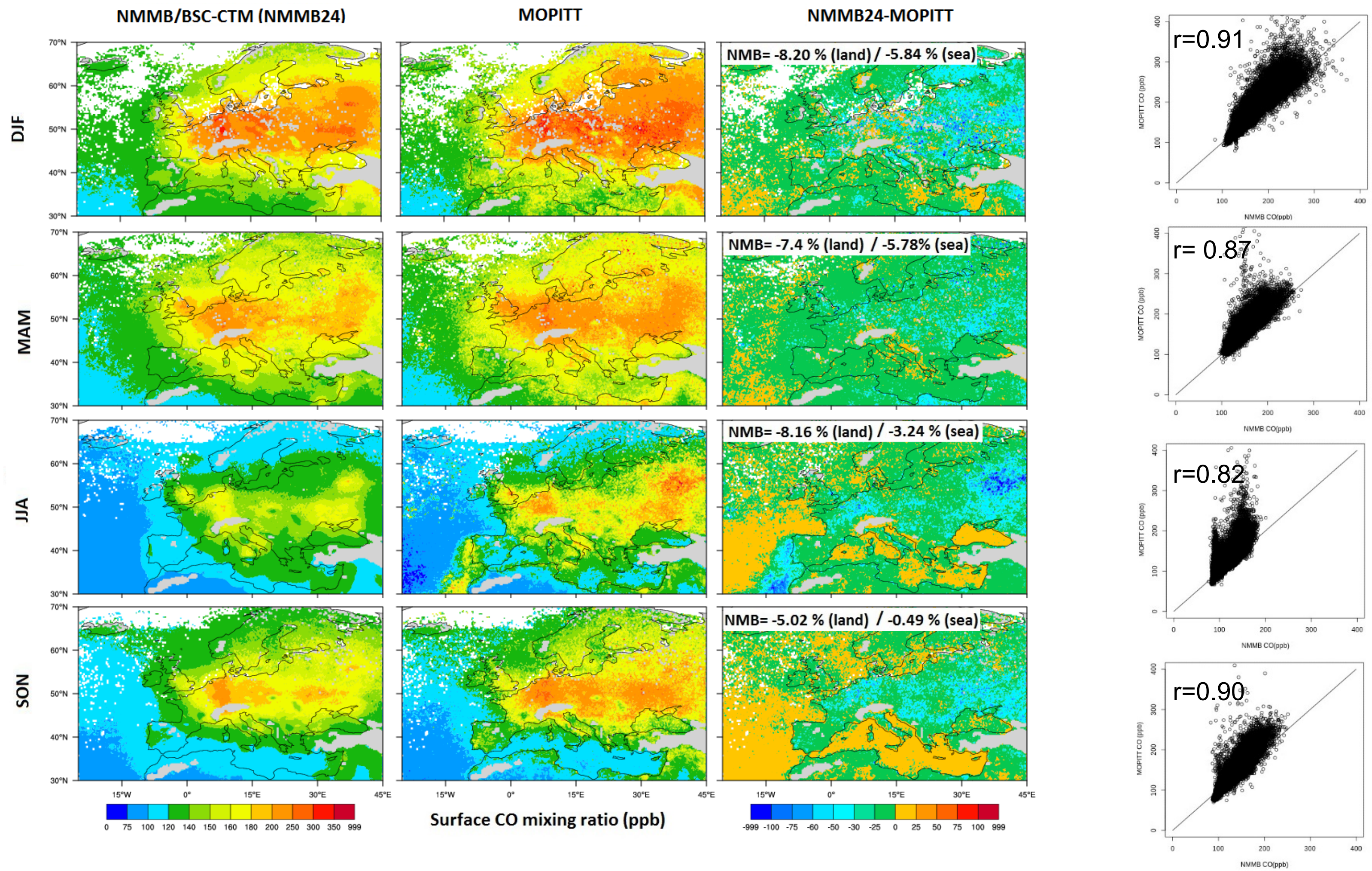
Comparison of modelled NO_2 VTC against satellite data (OMI) for (from top) winter (DJF), spring (MAM), summer (JJA) and autumn (SON)



(Badia and Jorba, 2014)

- Capturing higher NO_2 over the most polluted regions.
- **Over land:** Overestimate in big cities and underestimate in rural regions.
- **Over sea:** Overestimation in Mediterranean (Italy) and North seas -> shipping emissions or stability of marine boundary layer?

Comparison of modelled CO mixing ratio against satellite data (MOPITT) for (from top) winter (DJF), spring (MAM), summer (JJA) and autumn (SON)



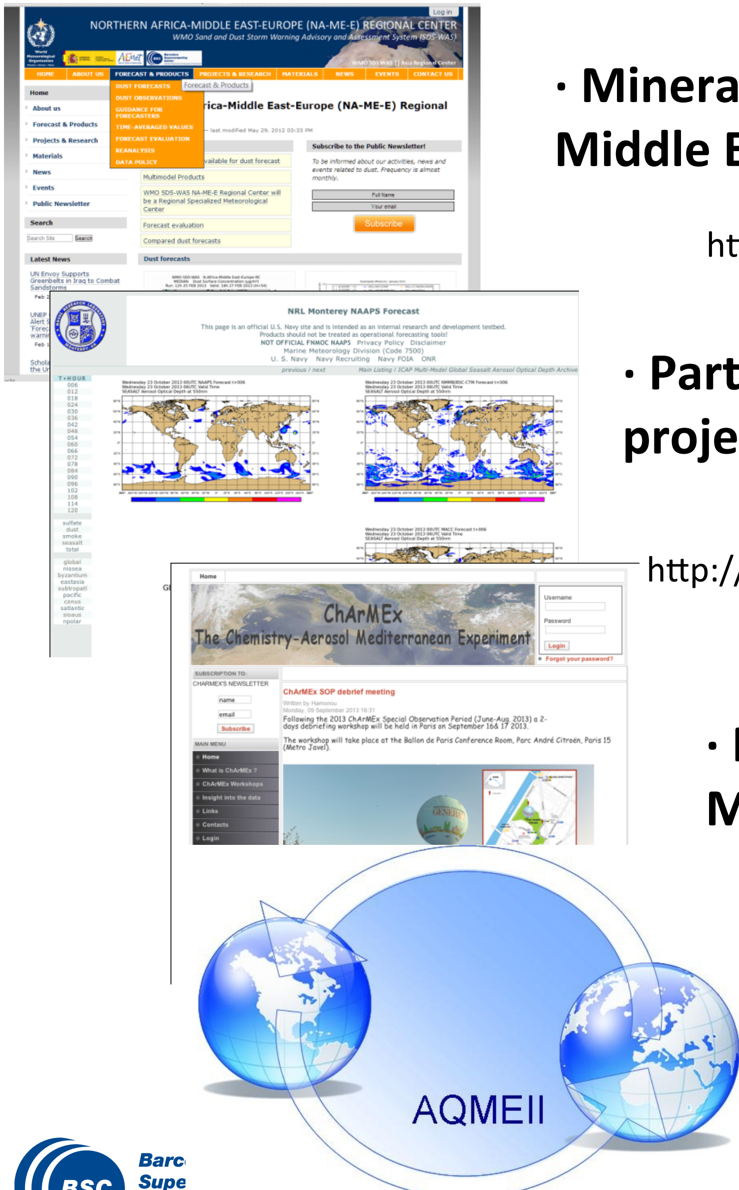
(Badia and Jorba, 2014)

- The pattern of emissions in central EU is well-captured.
- **Over land:** satellite evaluation confirms that there is a general trend to underestimate surface CO
- Summer underestimation due to no fires emissions (important fires in Russia and Portugal)

NMMB/BSC-CTM: Future Developments

- Coupling of chemistry gas-phase with a secondary aerosol scheme for LAM applications at high-resolutions.
- Evaluation 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).
- Evaluation of the online coupling of a volcanic ash module (Fall3D model, Folch et al., 2008)
- Implement effects of aerosols on meteorology:
  - aerosol-radiation
  - aerosol-clouds-radiation
- Explore methodologies for aerosol data assimilation

BSC aerosol and chemistry modelling collaborations



- **Mineral dust forecasts for SDS-WAS North Africa, Middle East and Europe portal**

  http://sds-was.aemet.es/

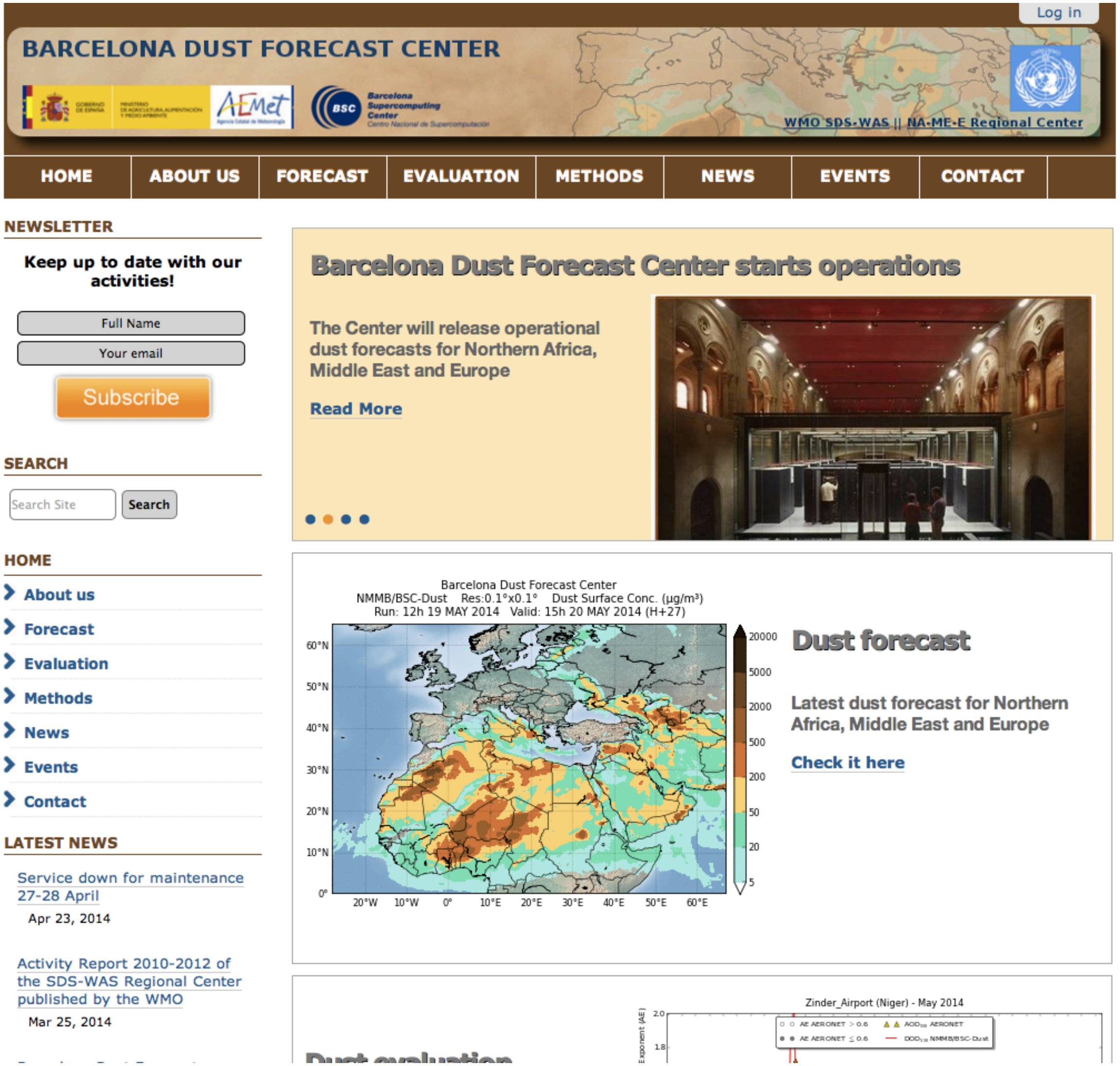
- **Participate in the ICAP global-model intercomparison project**

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

- **Participate in the Charmex Chemistry-Aerosol Mediterranean experiment**

- **Participate in the AQMEII on-line Air Quality model intercomparison project**

Barcelona Dust Forecast Center: **http://dust.aemet.es/**



First Specialized Center for Mineral Dust Prediction of the World Meteorological Organization

World Meteorological Organization
Weather • Climate • Water

Numerical forecasts based on the NMMB/BSC-CTM Dust component

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EXCELENCIA SEVERO OCHOA

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Thank you!

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www.bsc.es/projects/earthscience