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Aerosol Modelling activities and developments at the Earth Sciences Department

BSC update

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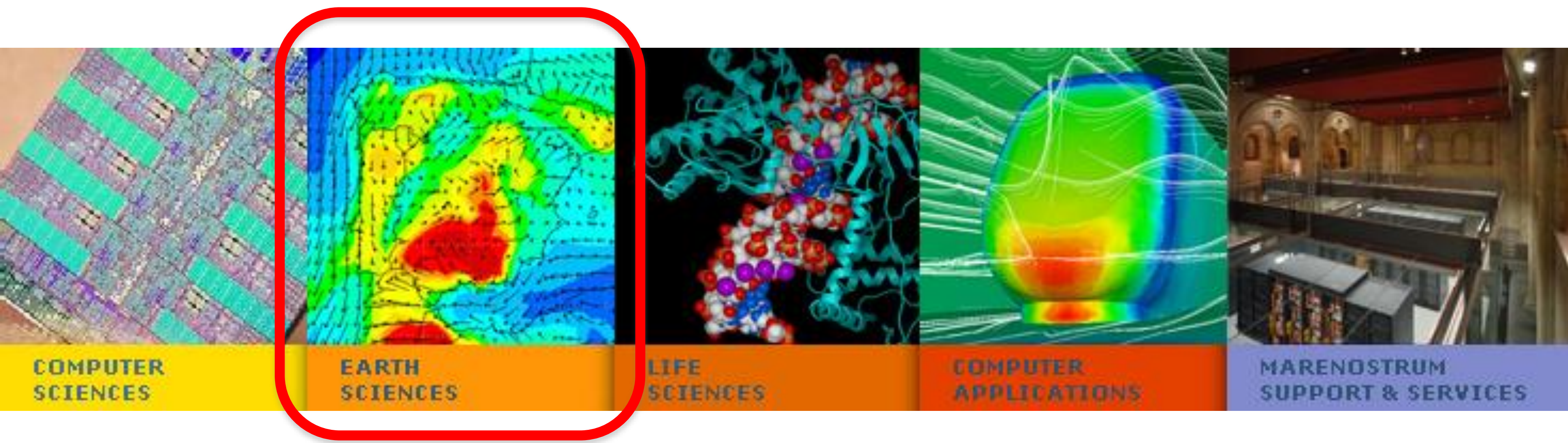
LL. Vendrell, V. Obiso, A. Badia, C. Pérez, A. Folch, A. Martí

Outline

- Description of the NMMB/BSC-CTM
- Aerosol modelling developments:
  - Mineral dust developments
  - Sea-salt sensitivity to resolution
  - Organic aerosol, black carbon, sulphate
  - Volcanic ash
- Gas-phase chemistry
- Future updates



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NMMB/BSC-CTM model description

NMMB/BSC-Chemical Transport Model

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- Multiscale: regional to global scales
- On-line coupled aerosols and chemistry allowing consistency and feedbacks

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)*
→ *(...)*

↕

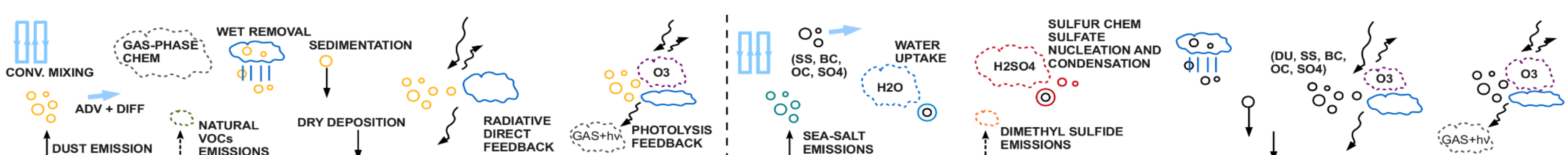
BSC Chemical Transport Model
(gas/aerosol variables: mass mixing ratios)

AEROSOLS

→ *Pérez et al. (ACP 2011)*
→ *Haustein et al. (ACP 2012)*
→ *Spada et al. (ACP 2013)*
→ *Spada et al. (AE 2014)*
→ *Spada et al. (GMD 2015 in prep)*

GAS-PHASE CHEMISTRY

→ *Jorba et al. (JGR 2012)*
→ *Badia and Jorba (AE 2014)*
→ *Badia et al. (GMD 2015 in prep)*



Aerosols I

- Mass-based approach. Dry sizes remain constant throughout the model simulation
- The wet size of hygroscopic particles changes with relative humidity for radiation and sedimentation calculations
- Dust: 8 size bins emitted as a function of friction velocity through a physically based dust emission scheme. Tested at global and regional scales (Northern Africa, Middle East and Europe)
- Sea-salt: 8 size bins emitted as a function of 10-m wind speed. 5 emission schemes available and thoroughly evaluated
- Black Carbon (BC): 2 tracers, one hydrophobic and one hydrophilic. Hydrophobic BC converted to hydrophilic with an e-folding time of 1.2 days (as in GOCART)
- Organic Matter (OM):
  - Primary Organic Matter (POA): 2 tracers, one hydrophobic and one hydrophilic. Hydrophobic OM converted to hydrophilic with an e-folding time of 1.2 days (as in GOCART)
  - Secondary organic aerosols (SOA): 4 gaseous and 4 aerosol-phase tracers. SOA produced by the reversible partitioning of the semi-volatile gaseous O3 oxidation products of isoprene and terpenes (Tsigaridis and Kanakidou, 2003; 2007). Anthropogenic SOA produced from toluene and xylene is under development

Aerosols II

- Sulfate (SO_4): 1 hydrophilic tracer, 4 additional prognostic tracers (SO_2, DMS, H_2O_2, H_2SO_4) and 3 online or climatological oxidants (OH, O_3, HO_2). Includes gas-phase oxidation of SO_2, DMS and H202 by OH, and aqueous-phase oxidation by H202 and O_3 (Sander et al., 2006, 2011)

- Nitrate (NO_3) and Ammonium (NH_4): as calculated by EQSAM thermodynamic equilibrium model but not tested yet (Metztger et al. 2002)

- Dry deposition from the bottom layer includes aerodynamic and surface resistance (Zhang et al., 2001)

- Gravitational settling follows the Stokes approximation including the Cunningham correction factor accounting for reduced viscosity for small aerosols

- In-cloud and below cloud scavenging from grid-scale (Ferrier) and sub-grid scale (BMJ) clouds

- Below cloud scavenging follows Slinn (1984) (directional interception, inertial impaction and Brownian diffusion)

- Vertical convective mixing follows the BMJ adjustment scheme (instead of a mass flux scheme)

- Radiation: RRTM SW/LW aerosol radiative feedback

- Optical properties: GADS refractive indexes (special for dust), Mie-scattering of spheres (Mischenko, 2000)

Gas-phase chemistry

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- OH, O3, HO2: for aerosol calculations we can use online gas-phase simulations or off-line climatologies
- Carbon-bond CBM-IV and CB05 mechanisms implemented (Gery et al., 1989; Yarwood, 2005)
- Coupled with Fast-J photolysis scheme (Wild et al., 2000)
- Mechanism implemented through KPP kinetic pre-procesor (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 as in CMAQ. Includes 51 chemical species and 156 reactions. Working version and thoroughly tested
- Stratospheric ozone: linear model Cariolle and Teyssèdre (2007) or Monge-Sanz et al. (2011)
- Dry deposition velocities depend on aerodynamic resistance, quasilaminar sublayer resistance and canopy or surface resistance (Wesely et al., 1986, 1989)
- Cloud chemistry: wet scavenging, mixing, and aqueous chemistry. Deposition follows Byun and Ching (1999) for grid-scale and subgrid-scale clouds

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Mineral Dust Module

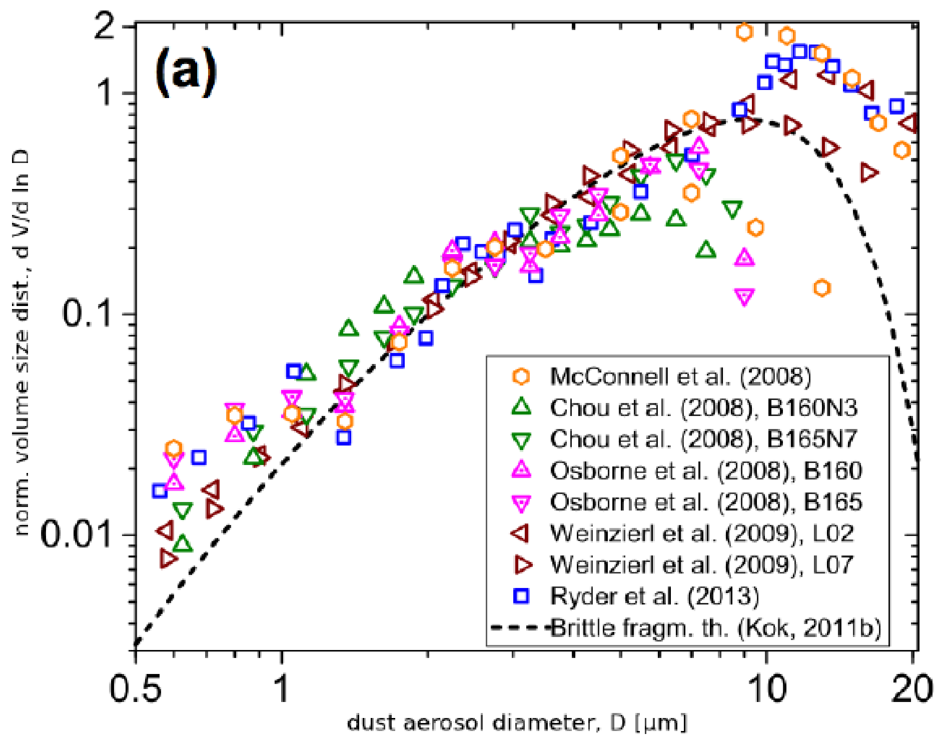
Kok's size distribution of emitted dust aerosols

applicable only when dust emission is predominantly due to the fragmentation of soil aggregates

$$\frac{dV_d}{d\ln D_d} = \frac{D_d}{c_V}\left[1 + \text{erf}\left(\frac{\ln(D_d/\bar{D}_s)}{\sqrt{2}\ln\sigma_s}\right)\right]\exp\left[-\left(\frac{D_d}{\lambda}\right)^3\right]$$

Its implementation into models has improved agreement against measurements in several regional and global models:

- Albani et al., 2014;
- Johnson et al., 2012;
- Nabat et al., 2012;
- Zhang et al., 2013.



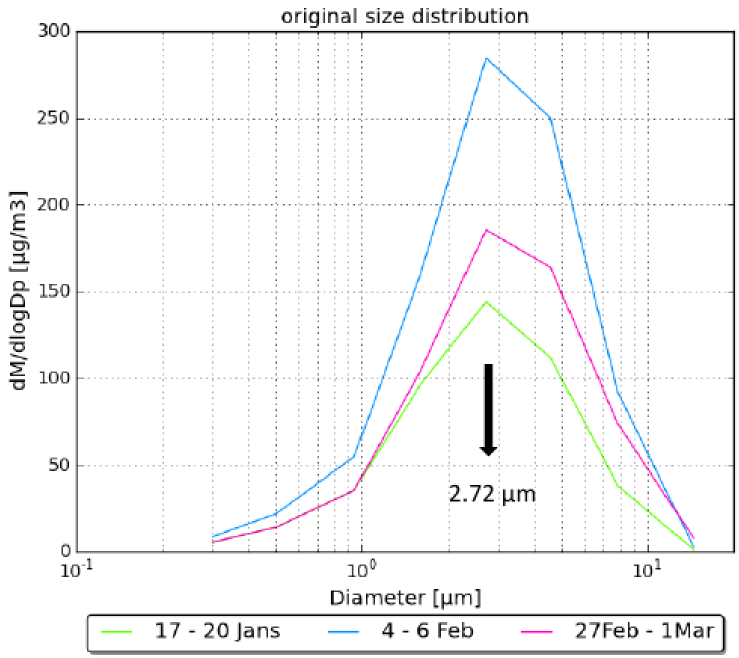
Kok (2011)
doi: 10.1073/pnas.1014798108

Extracted from Mahowald et al. 2013

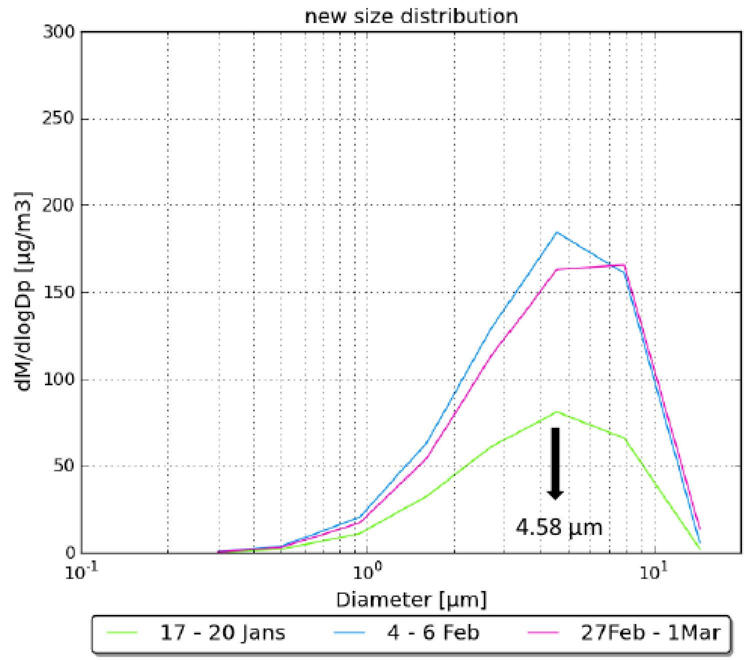
NMMB/BSC-CTM: Size distributions

Results over Praia, Cape Verde (surface) for 2011

D'Almeida (1986)

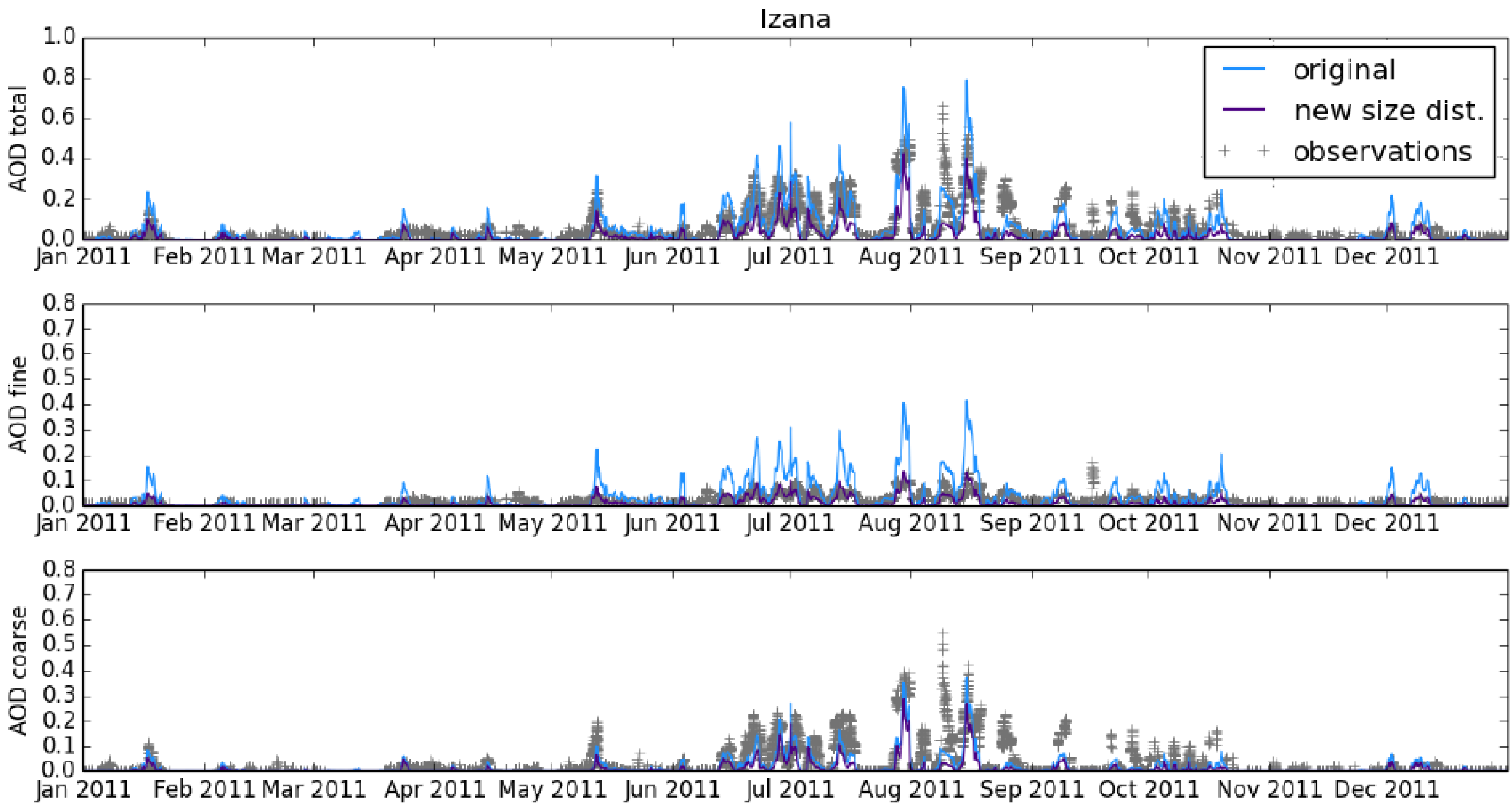


Kok (2011)



NMMB/BSC-CTM: Size distributions

Results over Izaña (AOD AERONET) for 2011



NMMB/BSC-CTM: Roughness length

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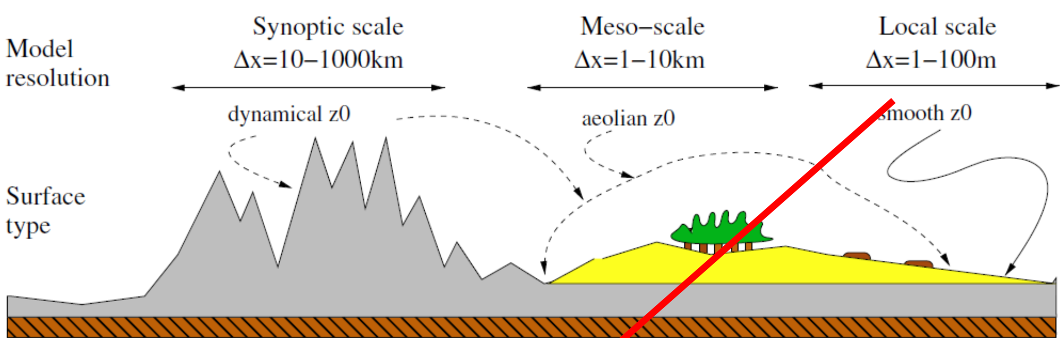
- **Threshold friction velocity u_{*thr}** is defined as the velocity above which soil particles begin to move in saltation flux
- Depends on **soil grain size, soil moisture and roughness (z_0)**

Threshold friction velocity over smooth surface and D_p the diameter of soil particles

$$u_{*thr}(D_p, z_0, w) = \frac{u_{*dry}(D_p)}{R(z_0, z_{0s})} \cdot H(w)$$

Moisture correction is introduced to account for the supression of soil erosion in wet soils

Drag partition correction
Z_0: roughness length
Z_{0s}: roughness length over smooth surfaces



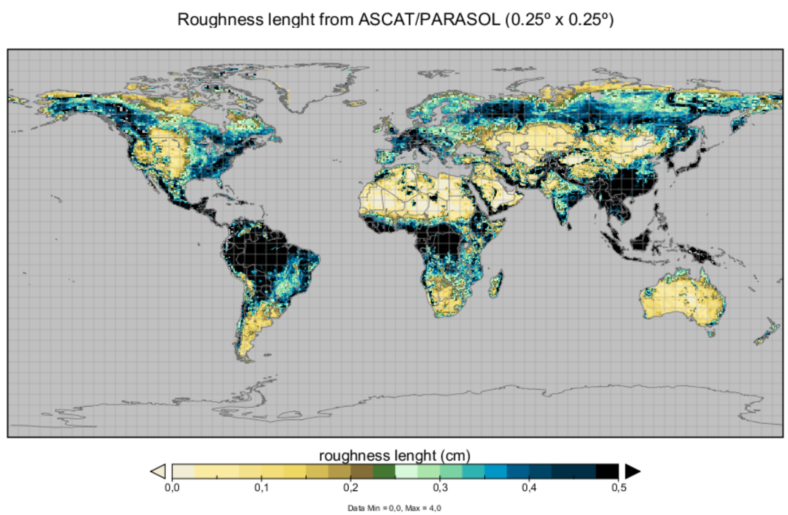
Extracted from Menut et al. (2013)

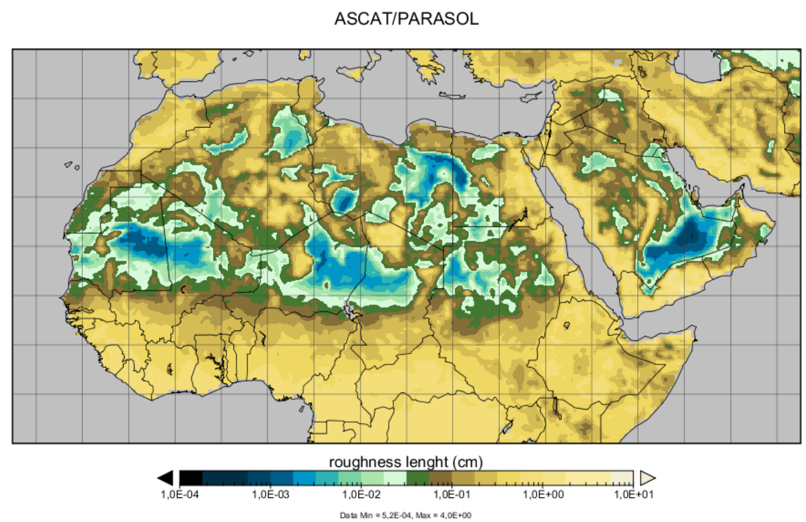
Figure 3. The roughness length definitions as a function of its use in local to global meteorological and dust transport models.

Satellite-derived roughness length (z_0) at global scale have emerged and provide the opportunity to use it in regional models (i.e. Menut et al., 2013)

NMMB/BSC-CTM: Roughness length

- Prigent et al. (2012) introduce new global map of the aeolian aerodynamic roughness length (Z_0) is derived from ASCAT/PARASOL, for arid and semi-arid regions.
  - *Z_0 derived from ASCAT backscattering (1999-2009) and PARASOL 865 nm (2005-2008)*
  - *Spatial resolution: ~ 6km x 6km (1/100º x 1/18º)*
  - *Valid range: 0 - 0.08 cm. They are calculated outside this range but their validity is questionable.*





NMMB/BSC-CTM: Dust mineralogy

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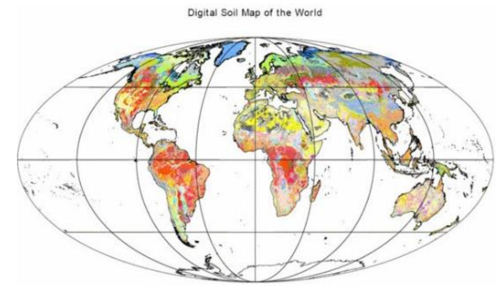
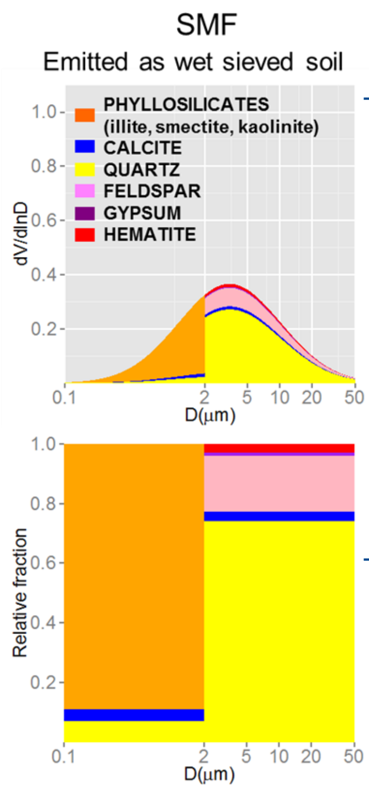
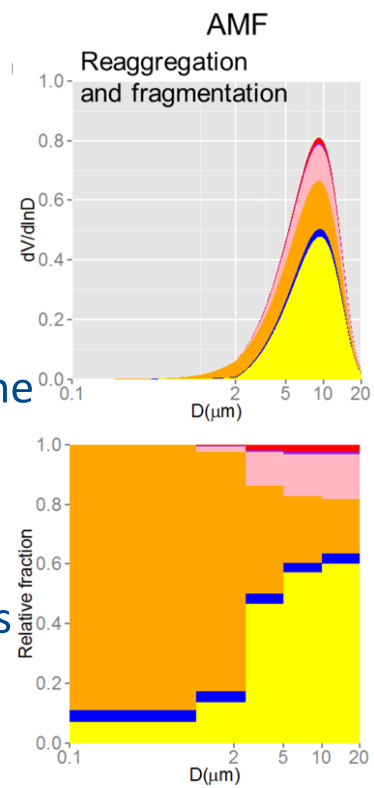


- Representing reaggregation of the original soil prior to wet sieving and fragmentation at emission is critical to estimate the global size-resolved dust mineral composition.
- Brittle fragmentation theory is a good approximation for models.



→ **Soil Mineral Fraction (SMF) (AMF) method** assumes aerosol mineral fractions match those of the soil.

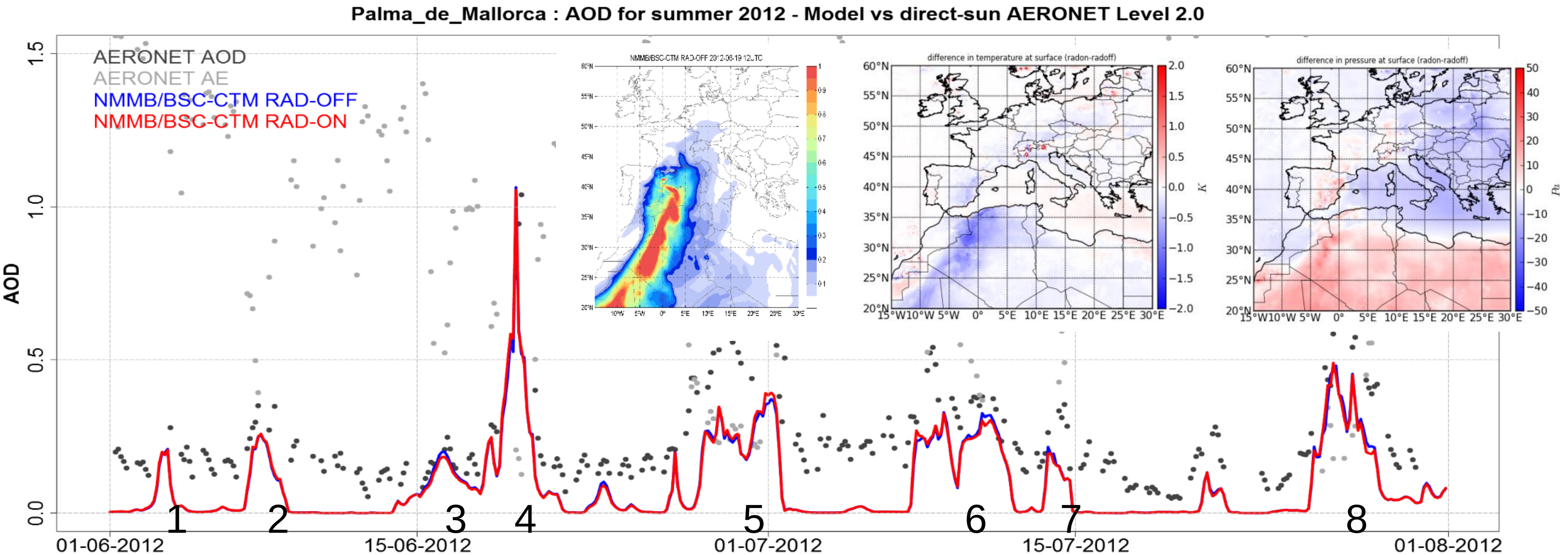
→ Implemented in most dust models



→ **Aerosol Mineral Fraction (AMF) method** described by Perlwitz et al. (2015a,b ACP)

→ Tested in NMMB/BSC-CTM model.

Interaction with meteorology: Direct effect of mineral dust

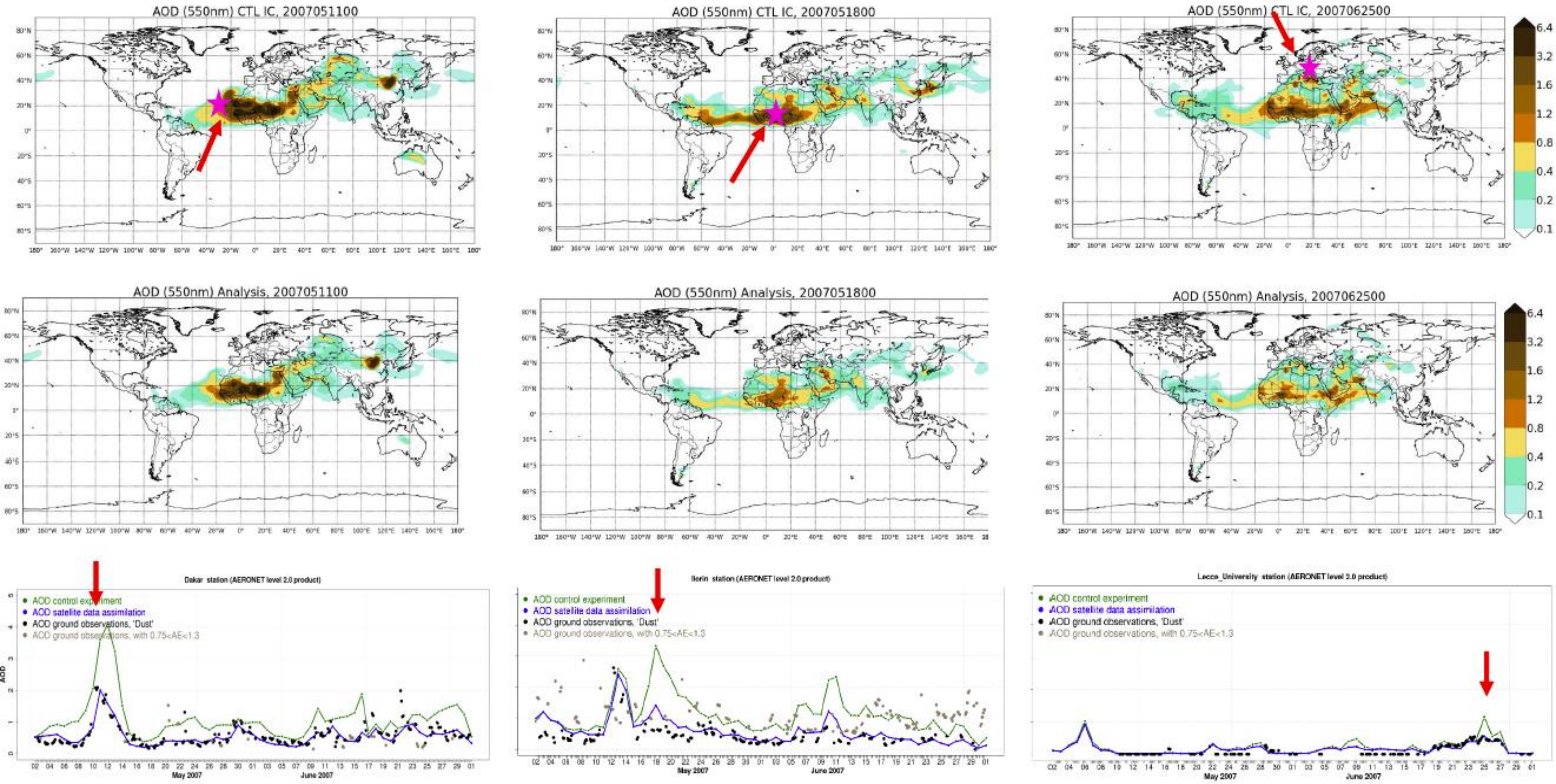


Event	1: 03-06	2: 07-06	3: 16-06	4: 19-06	5: 30-06	6: 10-07	7: 14-07	8: 27-07
ΔT_{sur} (K)	−0.037	−0.11	−0.023	−0.22	−0.10	−0.077	−0.071	−0.42
ΔP_{sur} (Pa)	−14.44	−3.95	−5.27	−3.17	−4.70	0.45	2.84	0.023
ΔQ_{sur} (gKg^{-1})	−0.061	−0.067	−0.053	−0.14	−0.099	0.004	−0.11	−0.15
$\Delta wind_{10}$ (ms^{-1})	−0.13	−0.11	0.10	−0.039	−0.059	0.013	−0.052	−0.13
ΔSW_{toa} (Wm^{-2})	15.47	14.03	9.56	54.21	26.80	18.20	7.11	34.06
ΔSW_{sur} (Wm^{-2})	−26	−23.19	−14.75	−133.20	−42.91	−24.87	−5.66	−54.17

NOTE: all the events with AOD>0.1 have been considered.

Data Assimilation for NMMB/BSC-CTM: Mineral Dust

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

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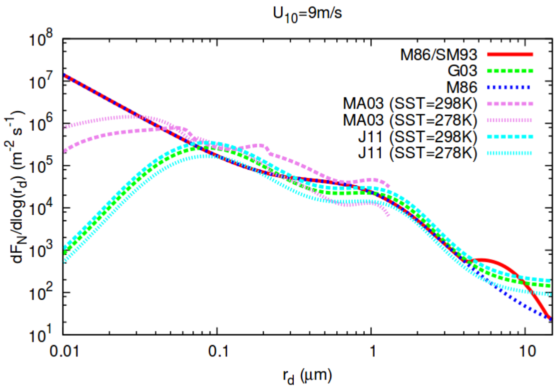
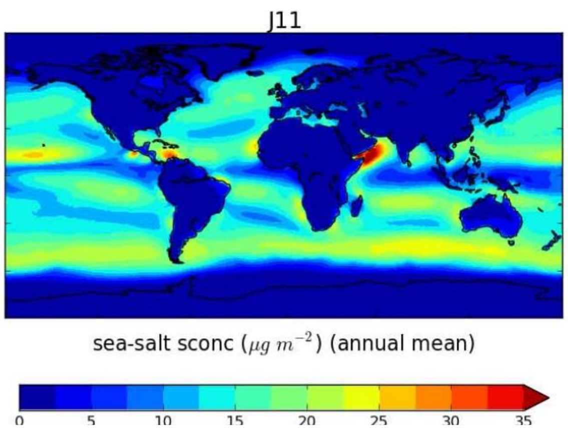
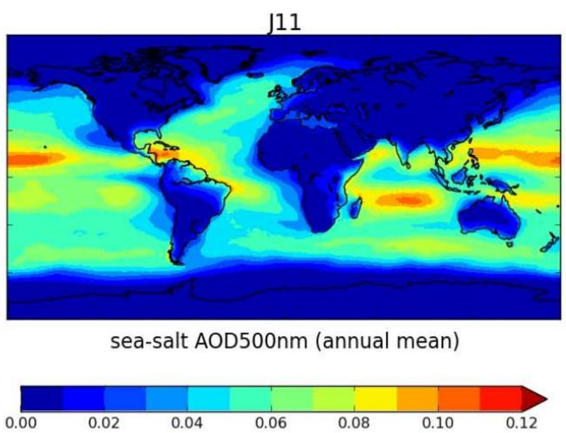
Sea Salt aerosol

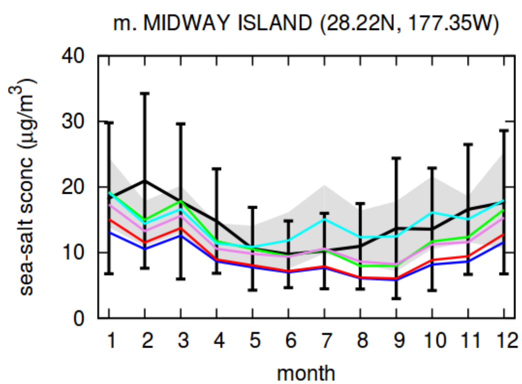
Sea-salt (global) Spada et al. (2013 ACP)

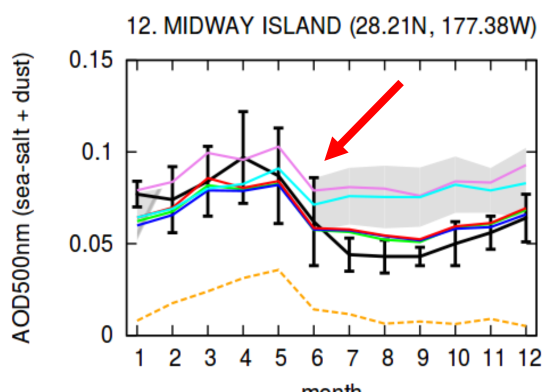


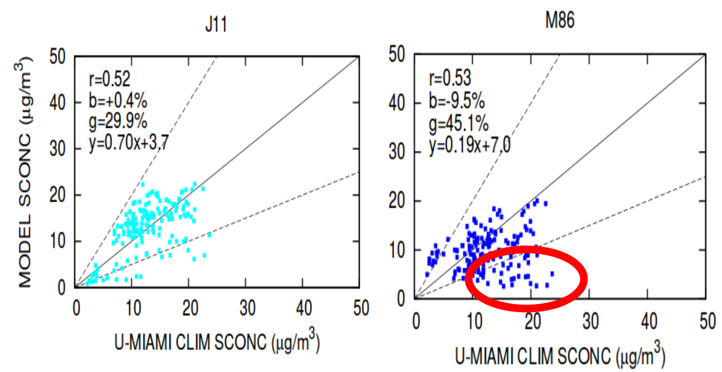


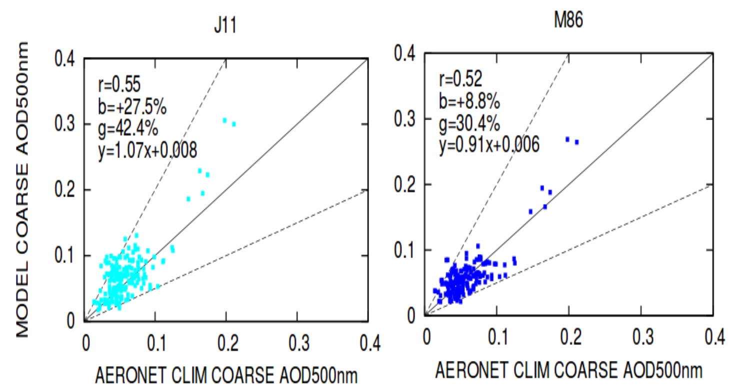


- Simulations between 2002 and 2006
- 5 online emission schemes implemented and tested (dependent on U10 and/or SST)
- Jaegle et al. (2011) best for surface concentrations globally (U. Miami stations) but tends to overestimate coarse AOD in tropical stations









Sea-salt (regional) Spada et al. (2015 AtmEnv)

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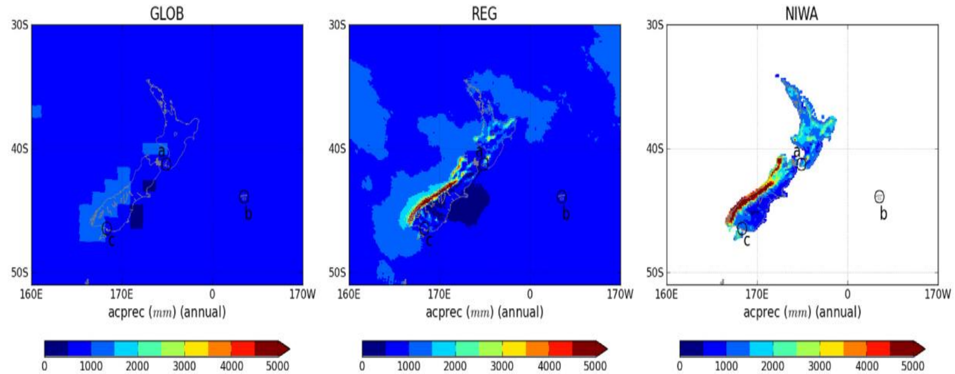
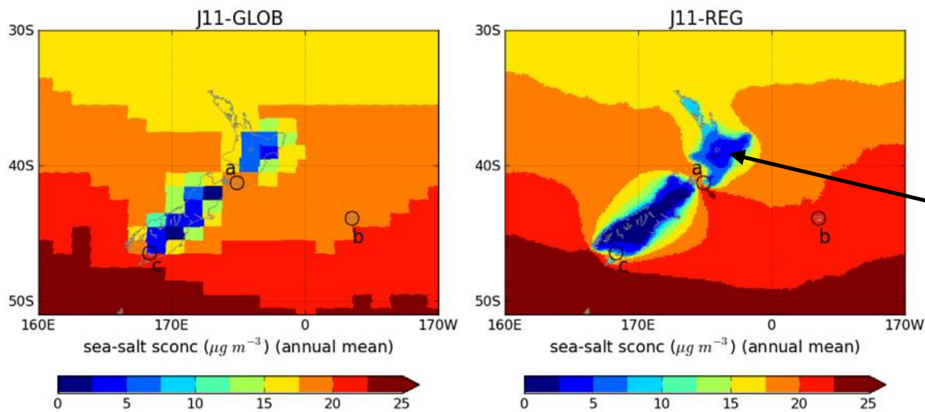
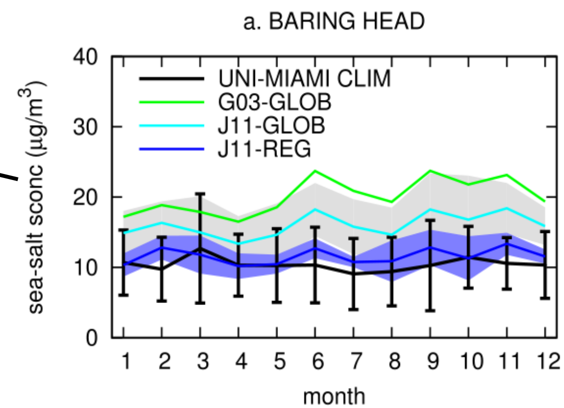
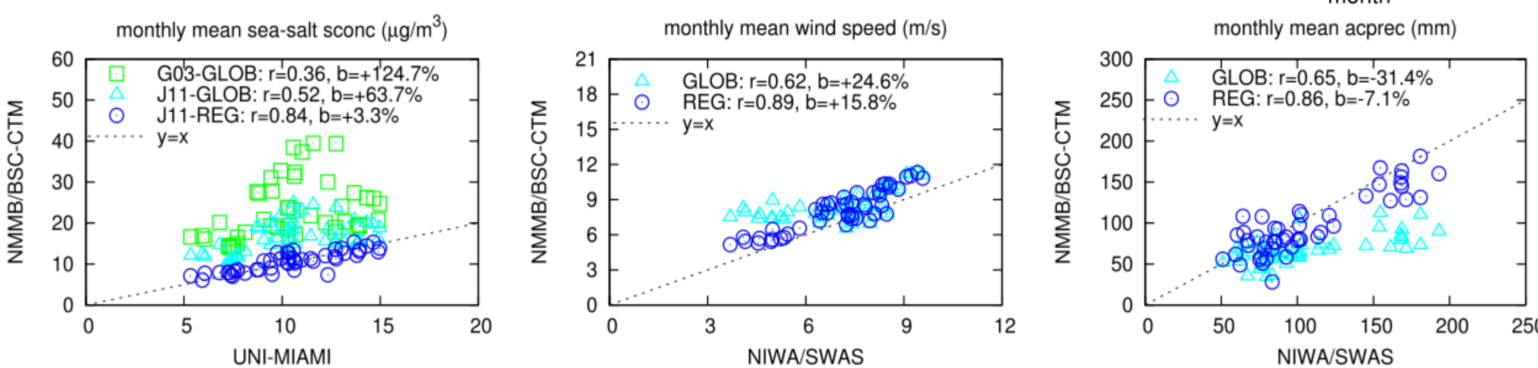


- Stations that unaffected by local surf conditions may no be considered representative of open ocean conditions from a meteorological point of view
- Enhancing resolution 1 deg to 0.1 deg over New Zeland: Sea-salt conc biases corrected in U. Miami stations surrounded by topography (factor of 2!)







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Organic aerosol, black carbon, sulphate

OA/BC/SO4 Spada et al. (2015 GMD in prep)

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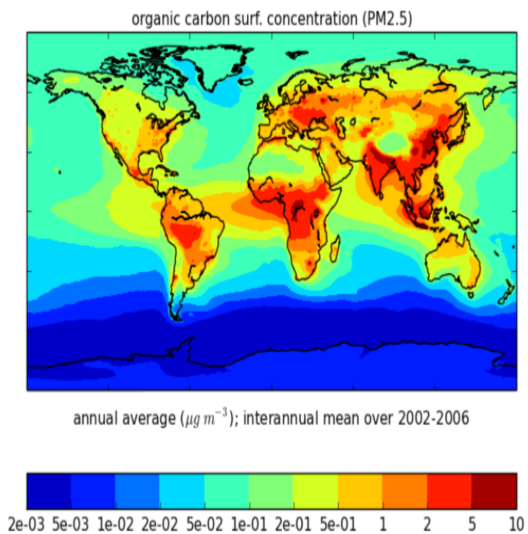
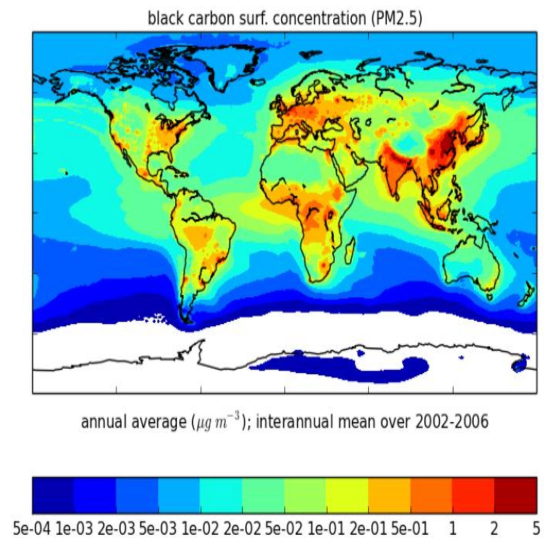
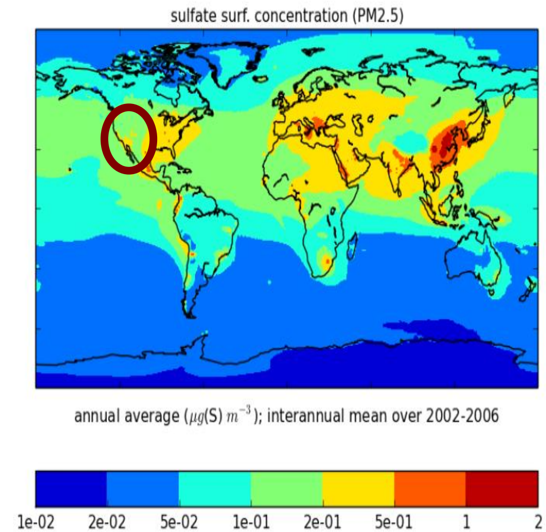
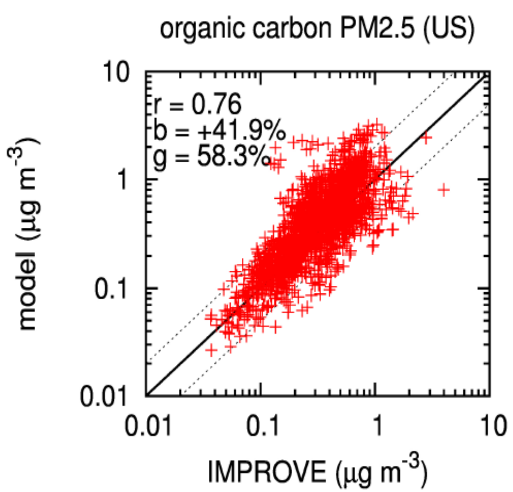
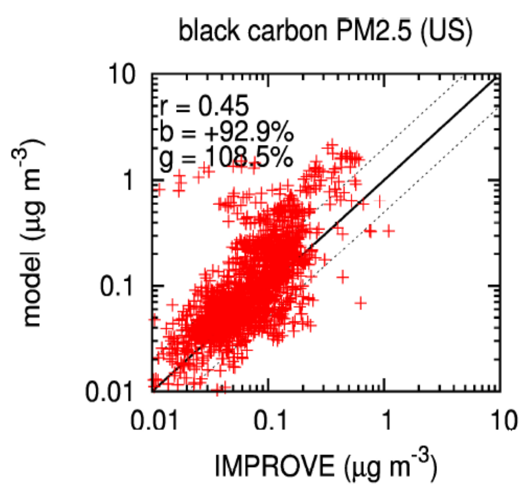
- *Anthropogenic and biomass burning emissions: ACCMIP (annual)*
- *Fires' inj. height: IS4F (monthly)*
- *Simulated years: 2002–2006 (monthly means eval.)*

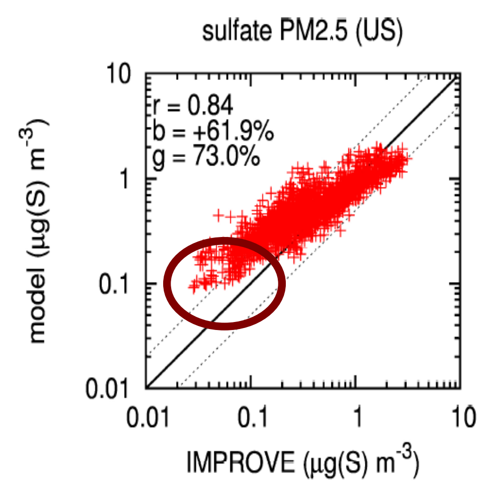








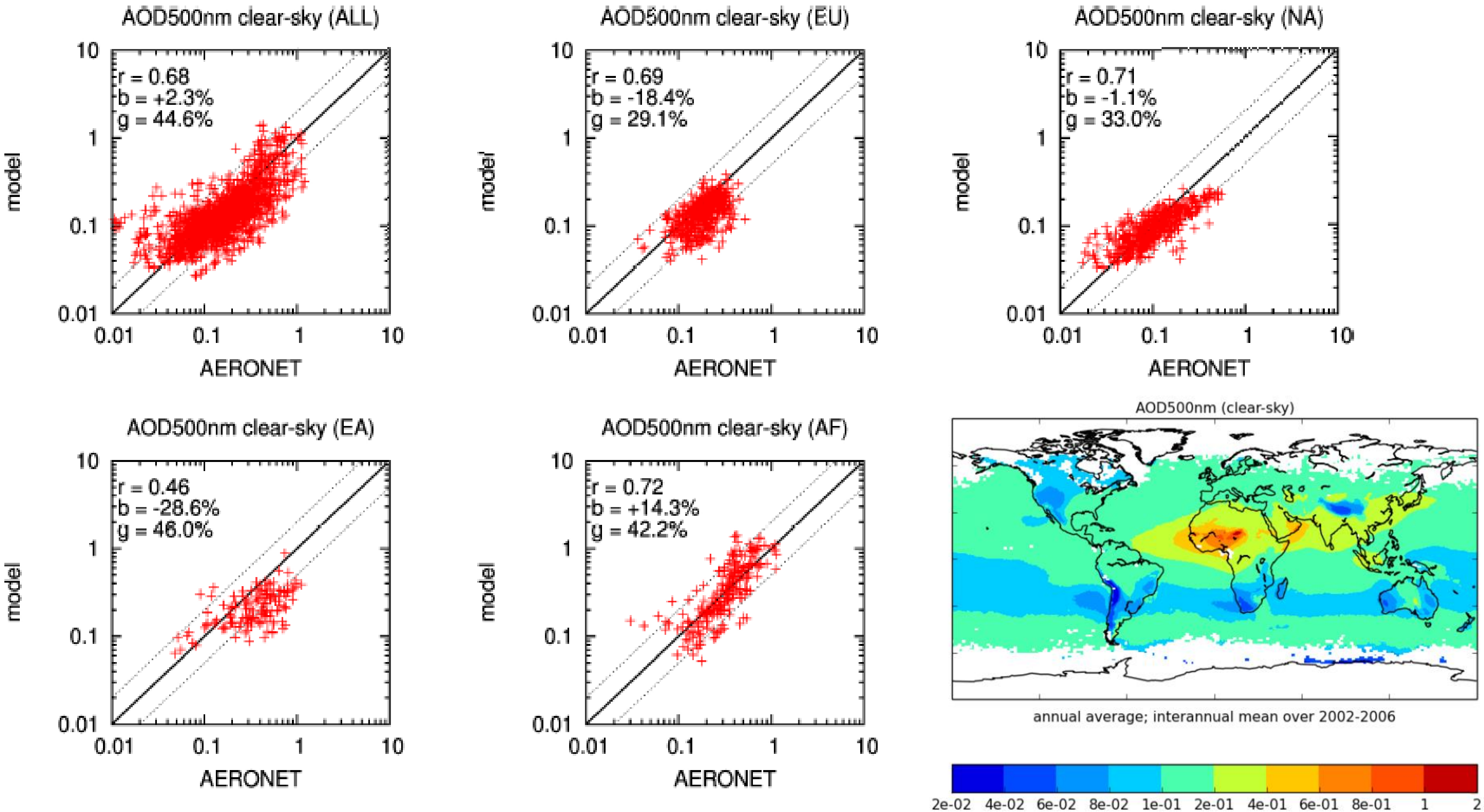




Clear sky AOD

Spada et al. (2015 GMD in prep)

Monthly data from 240 AERONET stations between 2002 and 2006



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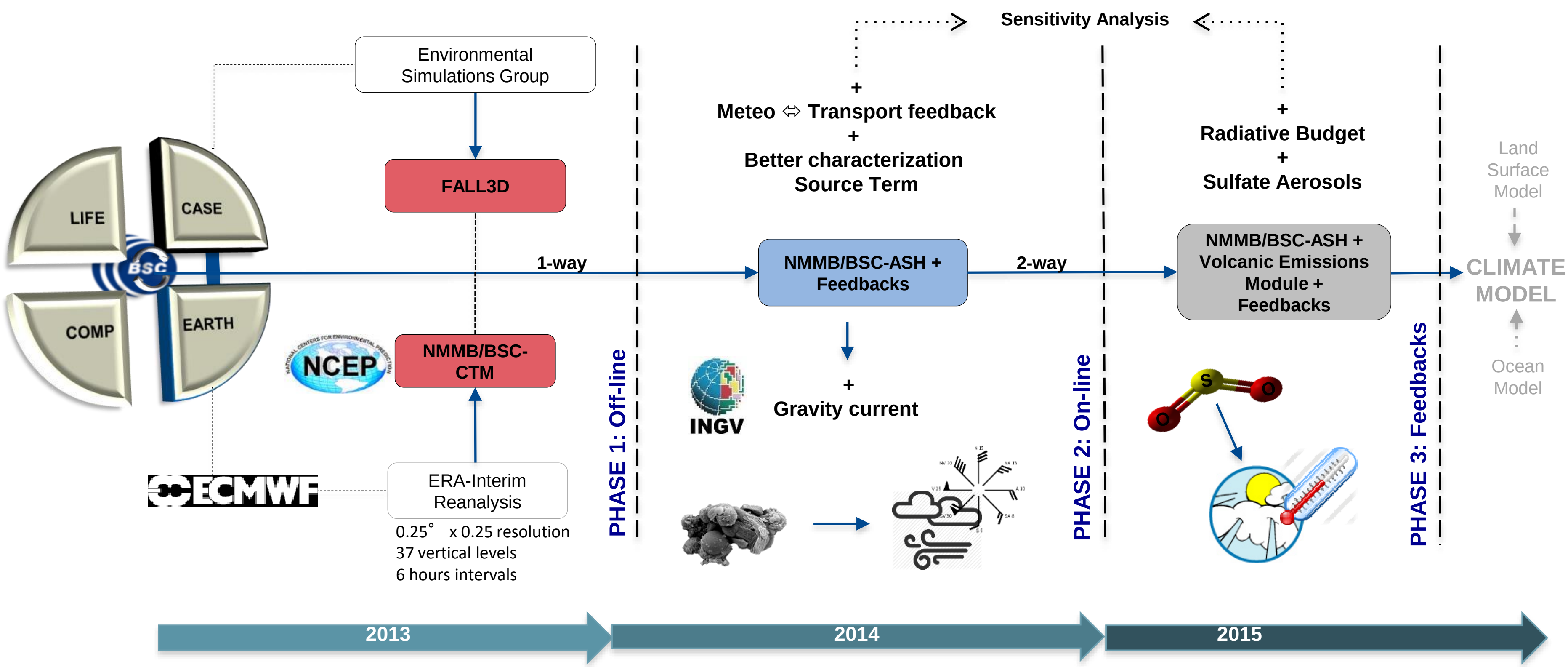
Volcanic Ash

Volcanic ash component

Martí et al. (2015 in prep)



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.

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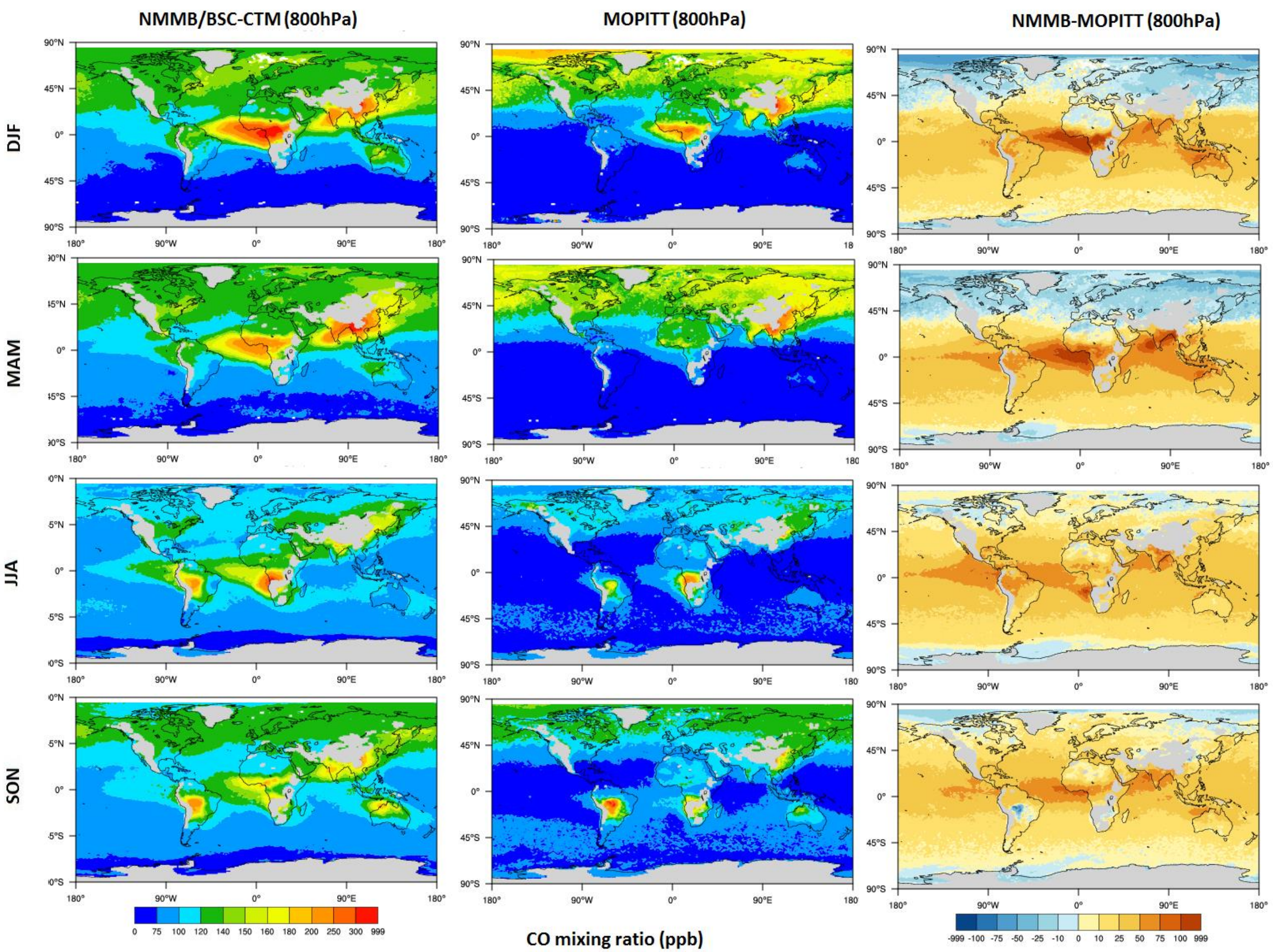
Gas-phase chemistry

Carbon Monoxide (CO)

Badia et al. (2015, GMD in prep)

- *Anthr. and BB emissions: ACCMIP*
- *Biogenic emissions: MEGAN*
- *No lightning emissions*
- *1 year spin-up*
- *2004 simulation*

Comparison with MOPITT (v5) at 800 hPa



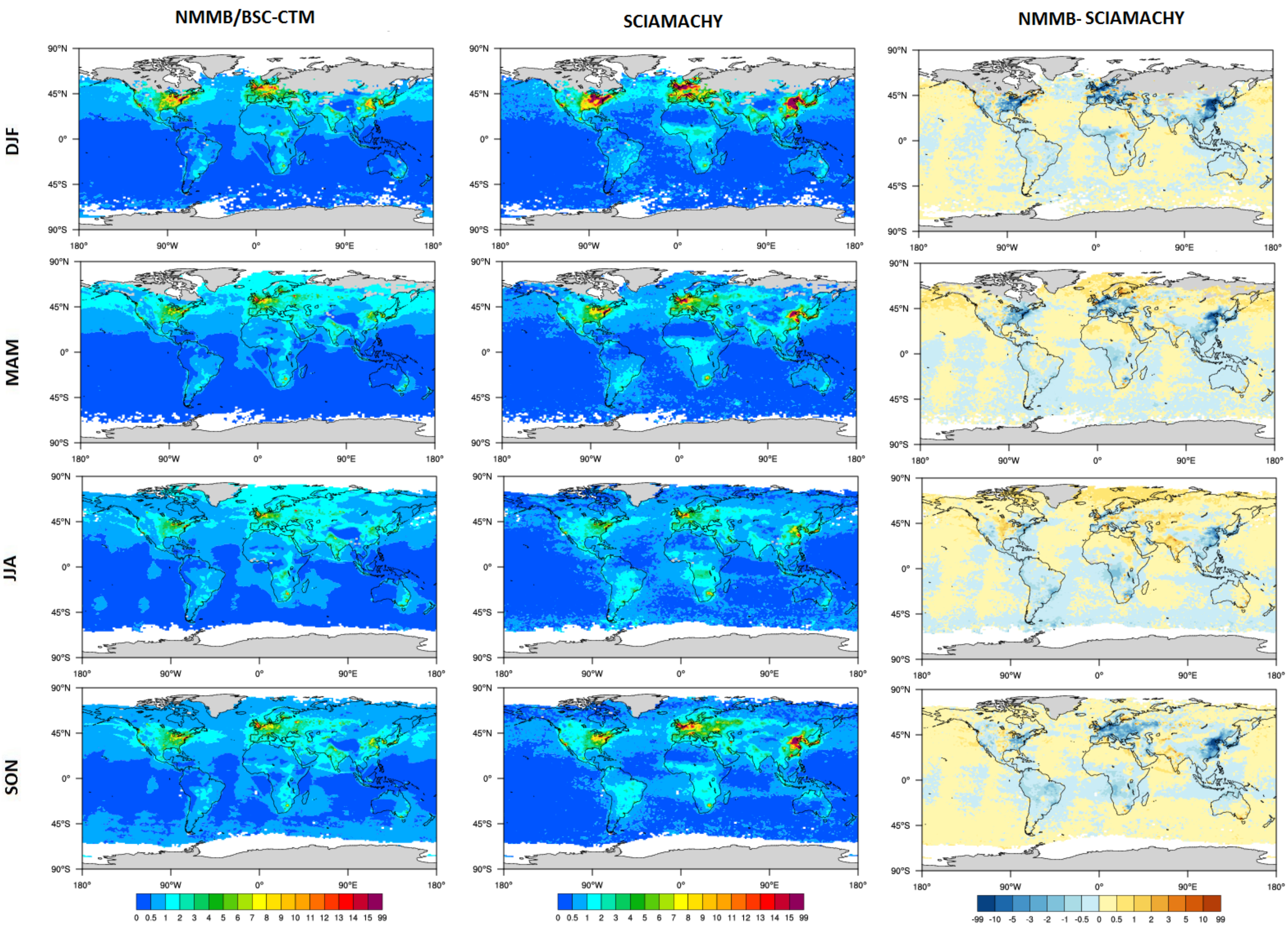
Strong overestimation over fire regions

Good agreement over polluted areas.

Need to implement attenuation of radiation due to aerosols in photolysis scheme.

NO_2 vertical tropospheric column

Badia et al. (2015, GMD in prep)



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Future plans

Future updates in ICAP

- Upgrades of the dust emission scheme
- Sea salt scheme based on Jaeglé et al. (2011)
- Data assimilation of MODIS AOD L3 product for mineral dust analysis
- Extending forecast to all aerosol components (BC/OM/Sulfate) to provide smoke and sulfate components
- Nesting implementation: Global to regional

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Thank you!

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