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Multiscale air quality with the NMMB/BSC Chemical Transport Model

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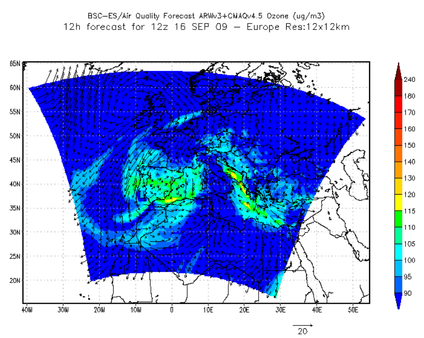
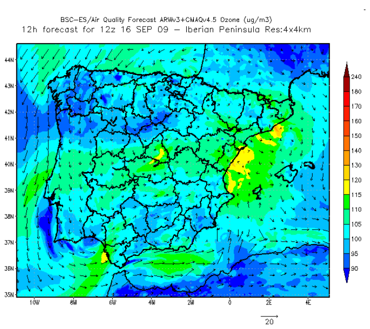
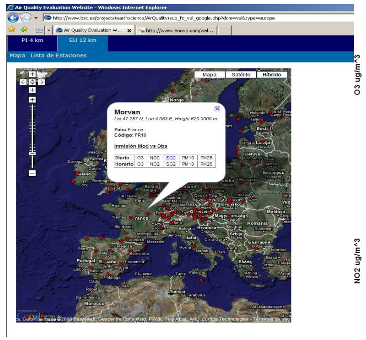
Motivation: BSC air quality modeling activities

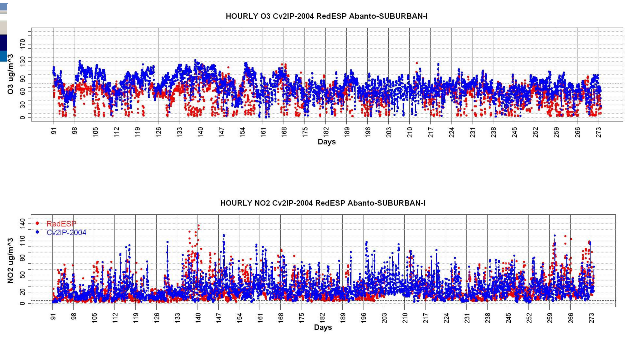
- CALIOPE daily forecast and verification

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





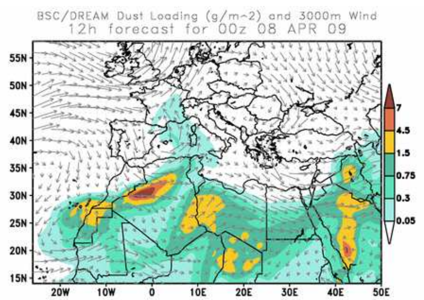


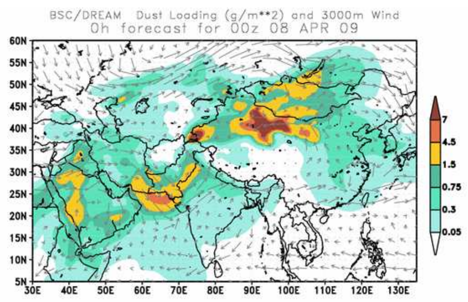


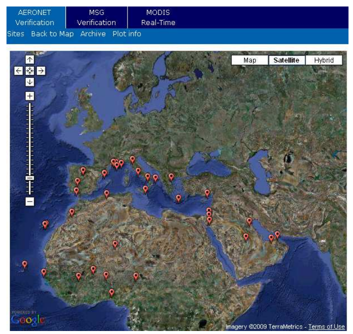
- BSC-DREAM8b daily forecast and verification

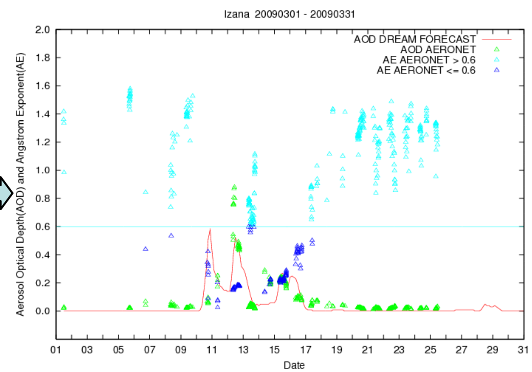
North Africa/Mediterranean - 1/3 x 1/3 degree resolution

Asia domain - 1/2 x 1/2 degree resolution









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

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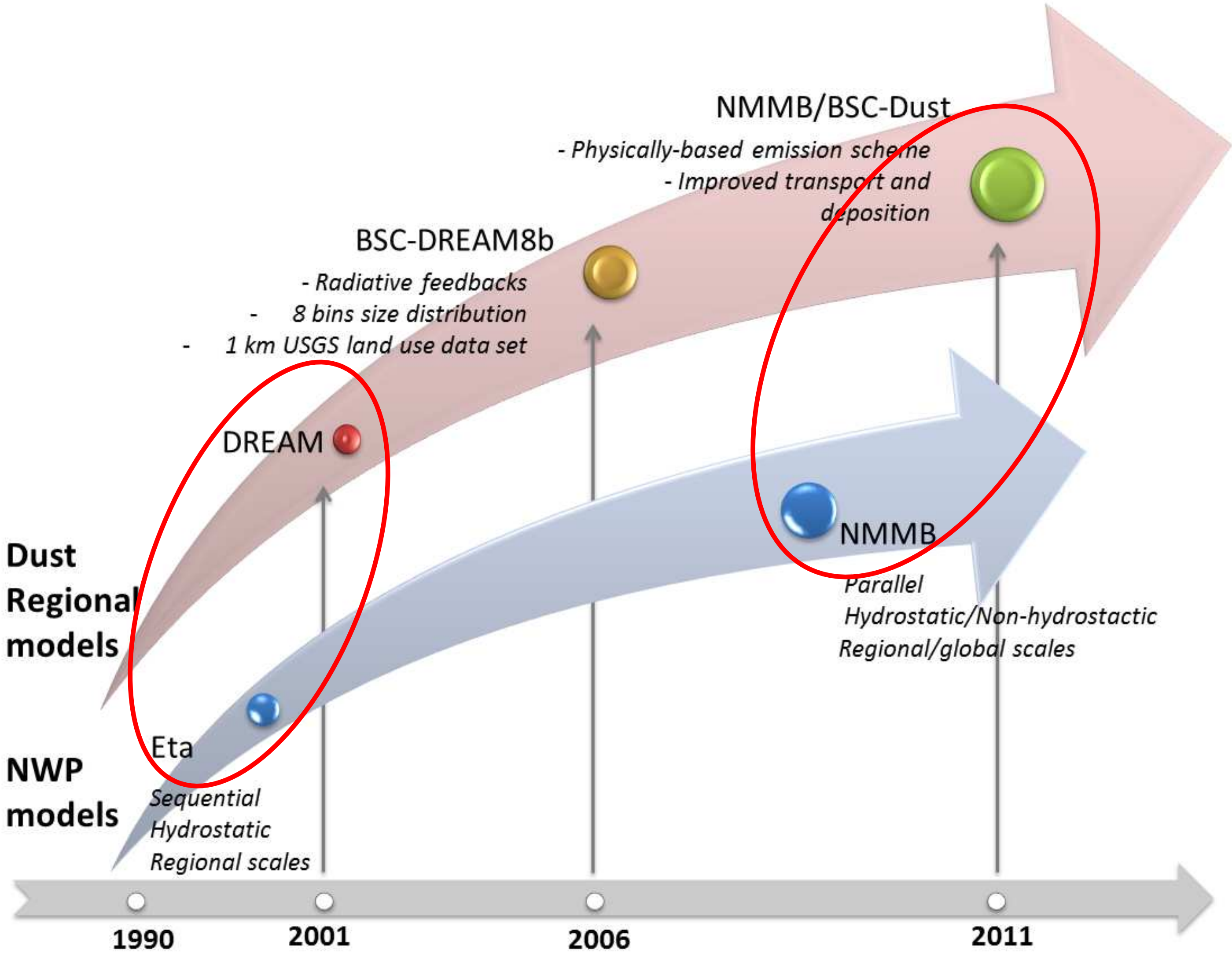
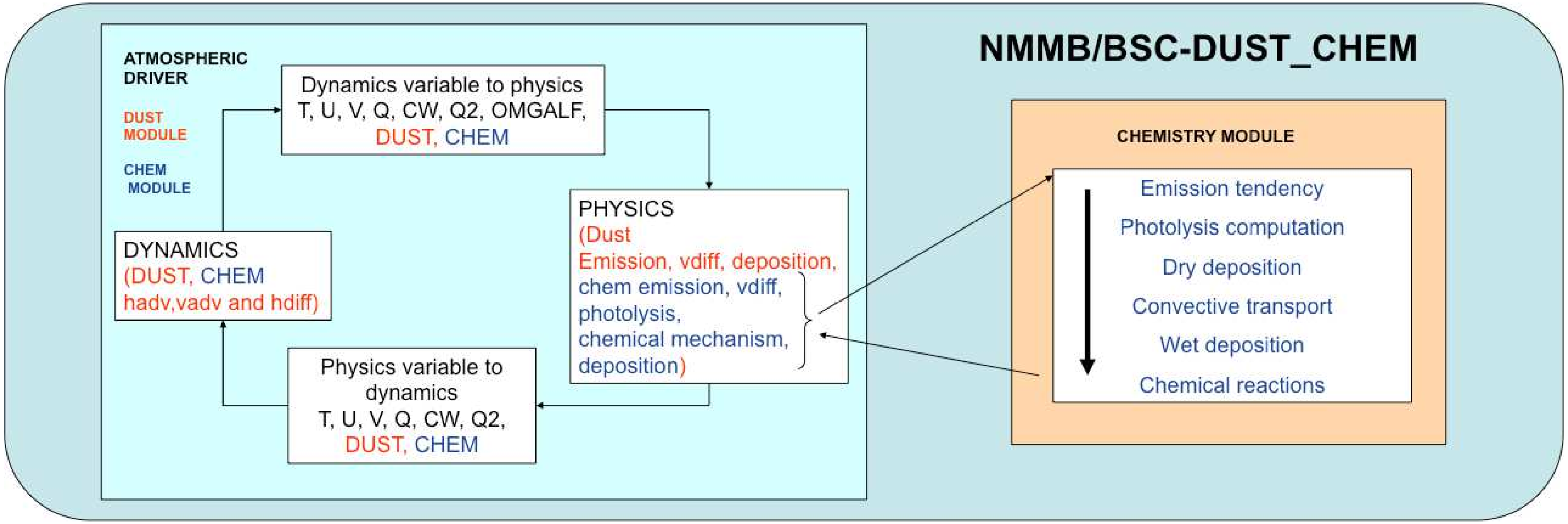
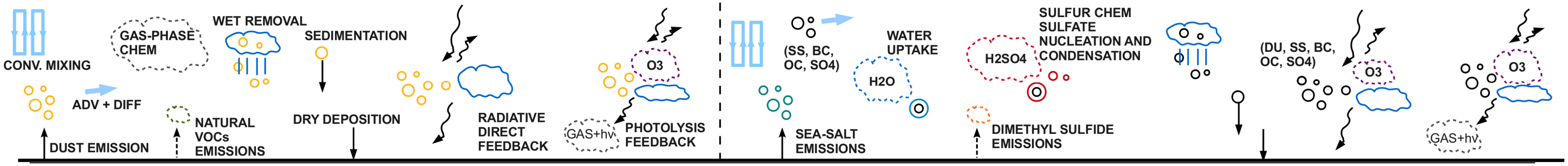
Historical evolution



NMMB/BSC-Chemical Transport Model

Embedding dust and chemistry processes within the meteorological core driver NMMB





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NMMB – Nonhydrostatic Multiscale Model on the B grid – Main characteristics
Under development at NCEP (Janjic, 2005; Janjic, 2007; Janjic, 2009; Janjic et al., 2011)

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

✓ Wide range of spatial and temporal scales (from meso to global)

✓ Regional and global domains (just a simple switch)

✓ Evolutionary approach,built on NWP experience by relaxing hydrostatic approximation
- ➢Favorable features of the hydrostatic formulation preserved

✓ The nonhydrostatic option as an add–on nonhydrostatic module

✓ No problems with weak stability on mesoscales

✓ Conservation of important properties of the continuous system

✓Arakawa B grid (in contrast to the WRF-NMM E grid)

✓Pressure-sigma hybrid

✓Improved tracer advection: Eulerian, positive definite, mass conservative and monotonic

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

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., 2012)
  - Complementing NMMB/BSC-DUST mineral dust aerosols
  - Same numerics like dust implementation
  - Inclusion of Sea Salt, BC, OC and sulfate
  - Implementation of feedbacks forseen

NMMB/BSC-CTM: gas-phase chemistry processes (Jorba et al., 2009-2012; Badia and Jorba, 2011)

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-CHEM O3 or climatology
- 7 bins wave-length (quick version)

$$J_i = \int_{\lambda_1}^{\lambda_2} F(\lambda)\,\sigma_i(\lambda)\,\phi_i(\lambda)\,d\lambda$$

$F(\lambda)$: actinic flux

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

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

- Tables of $\sigma_i(\lambda)$ and Φ_i (λ) 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-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
- Stratospheric ozone: linear model Cariolle and Teyssèdre (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 depositoin 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:

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

Scavenging:

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

$$\alpha_i = \frac{1}{\tau_{washout}\left(1 + \frac{TWF}{H_i}\right)} \qquad \tau_{washout} = \frac{\overline{W}_T \Delta z_{cld}}{\rho_{H_2O} P_r}$$

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

  - Wet deposition:

$$wdep_i = \int_0^{\tau_{cld}} \overline{m}_i^{cld} P_r\,dt$$

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NMMB/BSC-DUST: dust processes
(Pérez et al., 2008-2011; Haustein et al., 2009-2012)

NMMb/BSC-DUST emission scheme

→ Soil moisture effects [Fecan et al., 1999] (DREAM + NMMb-DUST)

$u_{*wet} = u_{*dry}\cdot\sqrt{1+1.21\cdot(w-w')^{0.68}}$ ⟹ $w' = (0.0014\cdot\%clay)^2 + 0.17\cdot\%clay$ w'=max amount of adsorbed water

→ Drag partition correction [Marticorena and Bergametti, 1995]

DREAM: /

NMMb-DUST: $u_{*total} = u_{*wet}\cdot\left(1-\frac{\ln(z_0/z_{0S})}{\ln(0.7\cdot(0.1/z_{0S}))^{0.8}}\right)^{-1}$

→ Threshold friction velocity [Bagnold, 1941; Iversen and White, 1982; Marticorena and Bergametti, 1995]

DREAM: $u_{*dry} = C\cdot\sqrt{2\cdot g\cdot R\frac{\rho_p-\rho_{air}}{\rho_{air}}}$

NMMb-DUST:

$$u_{*dry} = \sqrt{1+\frac{0.006}{\rho_p\cdot g\cdot D_k^{2.5}}}\cdot\sqrt{\frac{\rho_p\cdot g\cdot D_k}{\rho_{air}}}0.129\frac{1}{\sqrt{1.928\,\mathrm{Re}^{0.092}-1}} \quad (0.03<\mathrm{Re}\le 10)$$

$$u_{*dry} = \sqrt{1+\frac{0.006}{\rho_p\cdot g\cdot D_k^{2.5}}}\cdot\sqrt{\frac{\rho_p\cdot g\cdot D_k}{\rho_{air}}}0.129\cdot\left(1-0.0858\cdot e^{-0.0617\cdot(\mathrm{Re}-10)}\right) \quad (\mathrm{Re}>10)$$

→ Horizontal flux [White, 1979]

DREAM: Implicit in vertical flux

NMMB-DUST: $G = \frac{\rho_{air}}{g}u_*^3\cdot\sum_i\left(\left(1+\frac{u_{*total}}{u_*}\right)\cdot\left(1-\frac{u_{*total}^2}{u_*^2}\right)\cdot s_i\right)$ s_i=relative surface area of each soil fraction

→ Vertical flux [Shao et al., 1993; Marticorena and Bergametti, 1995; Tegen et al., 2002]

DREAM: $F_S = c\cdot\delta_{DREAM}\cdot u_*^3\cdot\left(1-\frac{u_{*total}^2}{u_*}\right)$

NMMb-DUST: $F_S = c\cdot\alpha\cdot\delta\cdot G$ ⟹ $(u_*\ge u_{*total})$

→ Viscous sublayer effects near the surface [Janjic, 1994] (DREAM + NMMb-DUST)

$F_{SZ0} = K_S'\cdot\frac{C_{LM}-C_0}{\Delta z}$ ⟹ $K_S' = \frac{1}{1+\omega}K_S$ K_S=diffusion coefficient; ω=weighting factor

NMMB/BSC-DUST: dust processes
(Pérez et al., 2008-2011; Haustein et al., 2009-2012)

→ Turbulent deposition [Giorgi, 1986] (DREAM + NMMb-DUST)

$$\upsilon_{dep} = \frac{1}{\frac{1}{\upsilon_{SL}} + \frac{1}{f_{B0}\cdot\upsilon_{IL}}}$$

$$\upsilon_{SL} = C_{D10}\cdot U_{10}\frac{\sqrt{C_{D10}}}{\sqrt{C_{D0}} - \sqrt{C_{D10}}}$$ ⟹ layer between surface and 10m

$$\upsilon_{IL} = G\cdot\sqrt{C_{D10}\cdot u_*}$$ ⟹ at top at viscous sublayer

→ factor G accounts differently for surface with turbulent regime and surface covered by vegetation
→ in the latter case accounting for Brownian diffusion, interception, impaction and small vegetation elements

→ Gravitational settling [Giorgi, 1986]

DREAM: $$v_g = \frac{2\cdot g\cdot \rho_k \cdot R_k^2}{9\cdot \nu}$$

NMMb-DUST: $$v_g = \frac{2\cdot g\cdot \rho_k \cdot R_k^2}{9\cdot \nu} Cc$$

$$Cc = 1 + \frac{2\cdot\lambda}{R_k}\left(1.257 + 0.4\cdot e^{\frac{-0.55\cdot R_k}{\lambda}}\right)$$ Cunningham correction

→ Grid scale precipitation [Slinn, 1983; 1984]

DREAM: Simple below cloud wasout ratio for grid-scale precipitation (Zhao microphysics)

NMMb-DUST: **In-cloud scavenging** from grid-scale clouds and **Below-cloud scavenging** from grid-scale precipitation (snow and rain) (Ferrier microphysics)

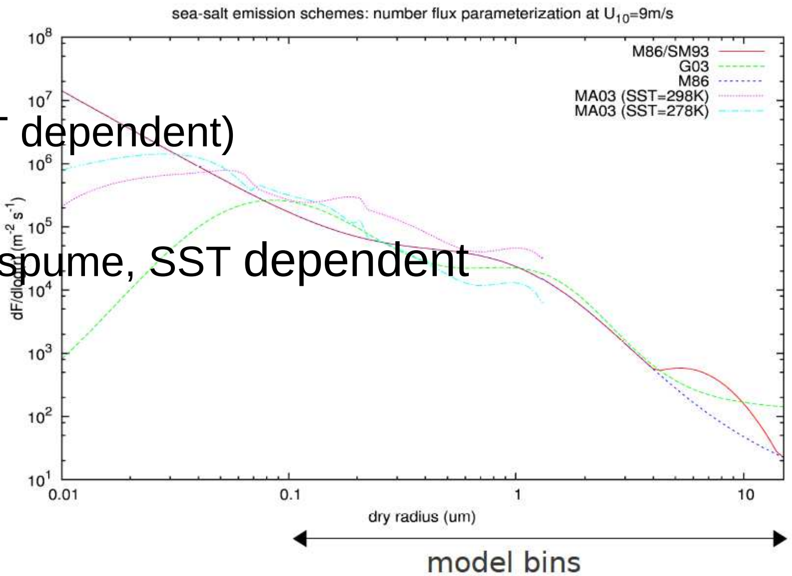
→ Convective precipitation [Loosmore and Cederwall, 2004]

DREAM: below cloud wasout ratio for convective precipitation (Betts-Miller-Janjic)

NMMb-DUST: **In-cloud and below-cloud scavenging** for convective precipitation (Betts-Miller-Janjic)

NMMB/BSC-CTM: Sea Salt processes (Spada et al., 2012)

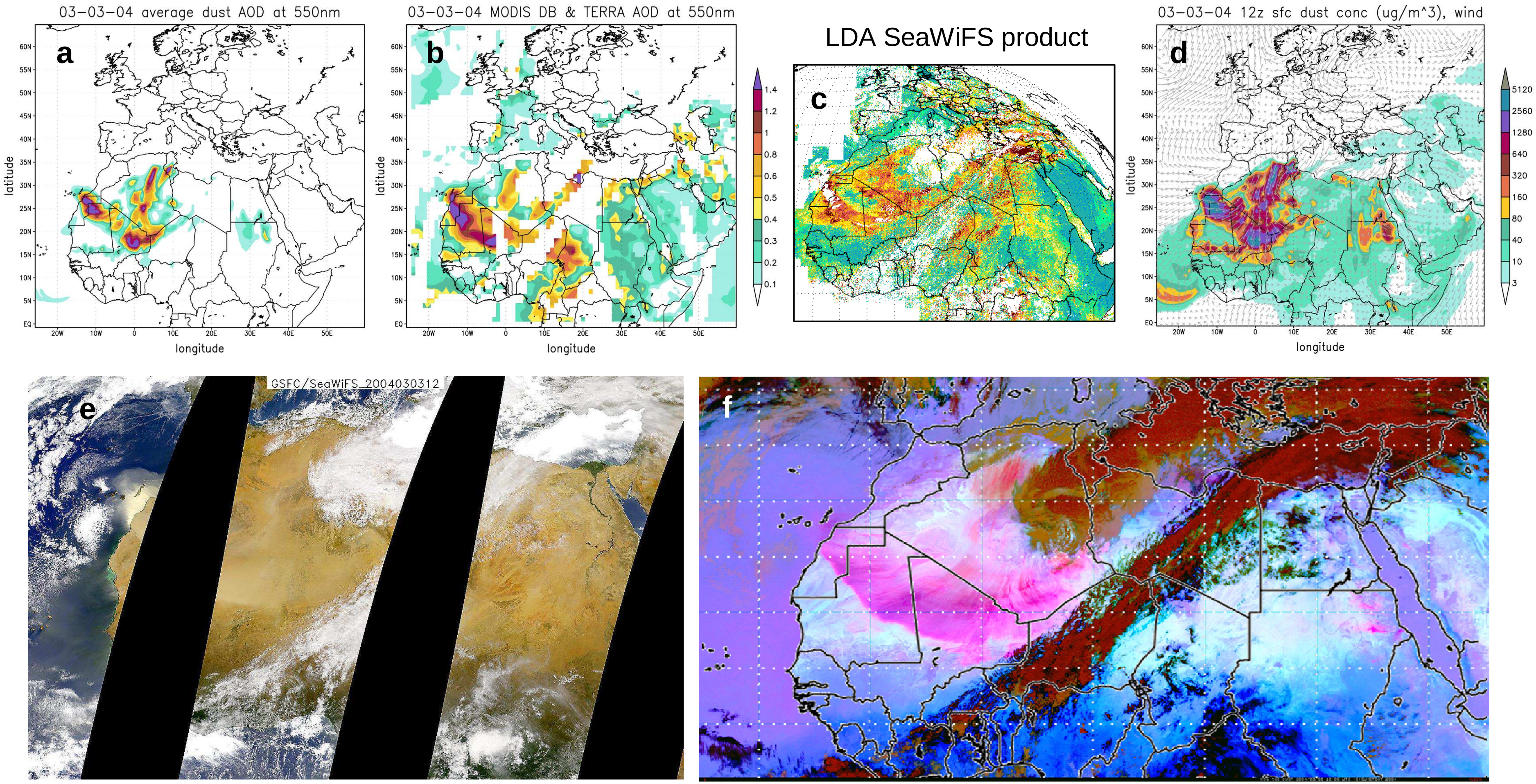
- Sectional approach – 8 bins for coarse and fine SSA
- Assumed dry density of 2160 kg/m^3, solubility factors derived from Zender et al. (2003)
- Hygroscopic growth following Chin et al. (2002)
  - Affecting gravitational settling, dry and wet deposition
- Different open-ocean sea-salt emission schemes implemented and tested.
  - Monahan et al. (1986) -> bubbles
  - Gong (2003) -> bubbles
  - Smith et al. (1993) -> bubbles, spume
  - Martensson et al. (2003) -> bubbles (SST dependent)
  - Combined M86/SM93 -> bubbles, spume
  - Combined MA03/M86/SM93 -> bubbles, spume, SST dependent



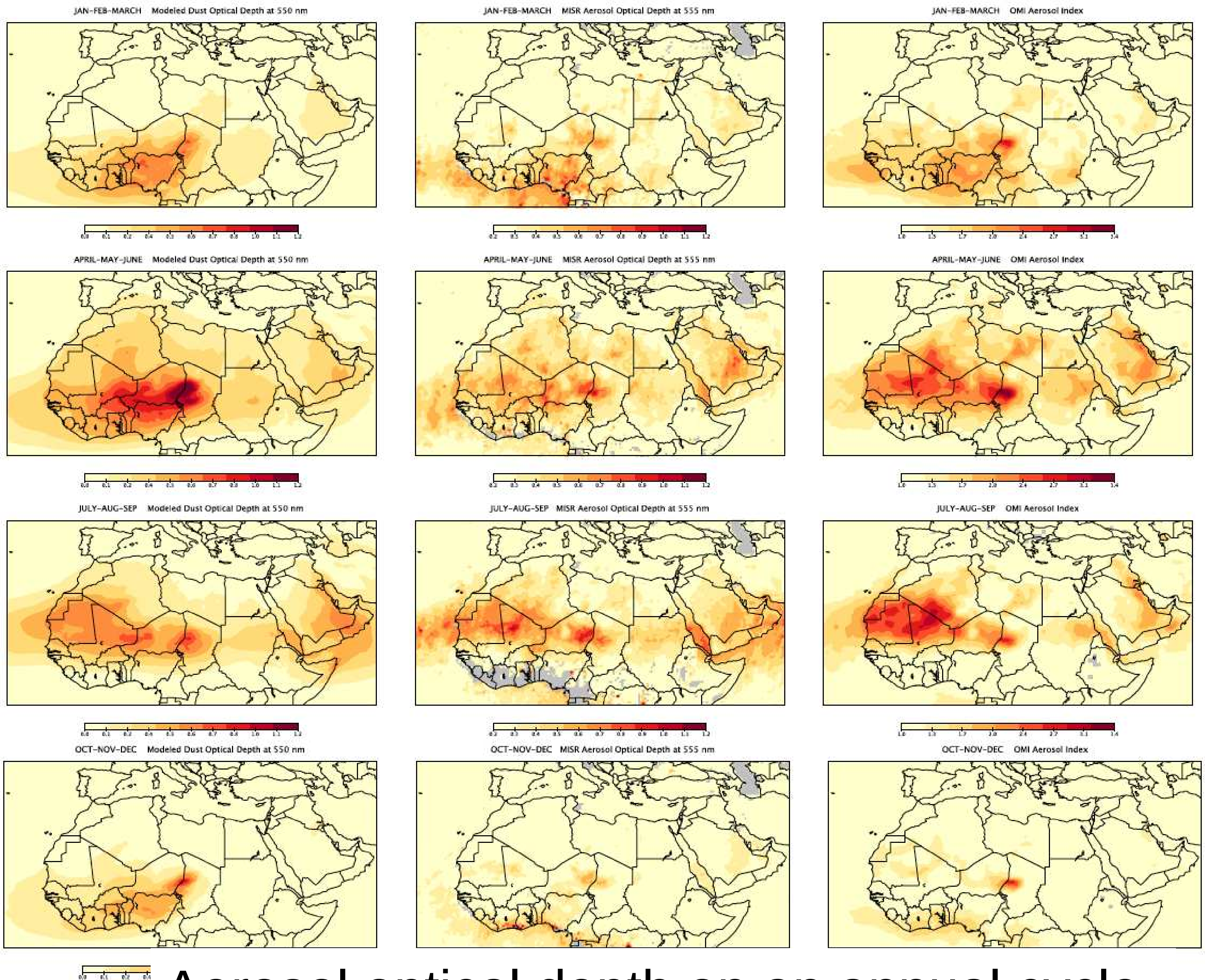
- Results and evaluation works
  - Dust
  - Gas phase chemistry
  - Sea salt

Results: Dust model

- Global and regional annual simulations evaluated with:
  - Aeronet sun-photometer networks
  - LIDAR vertical profiles
- Several satellite products
- Surface concentrations
- Emission and deposition fluxes



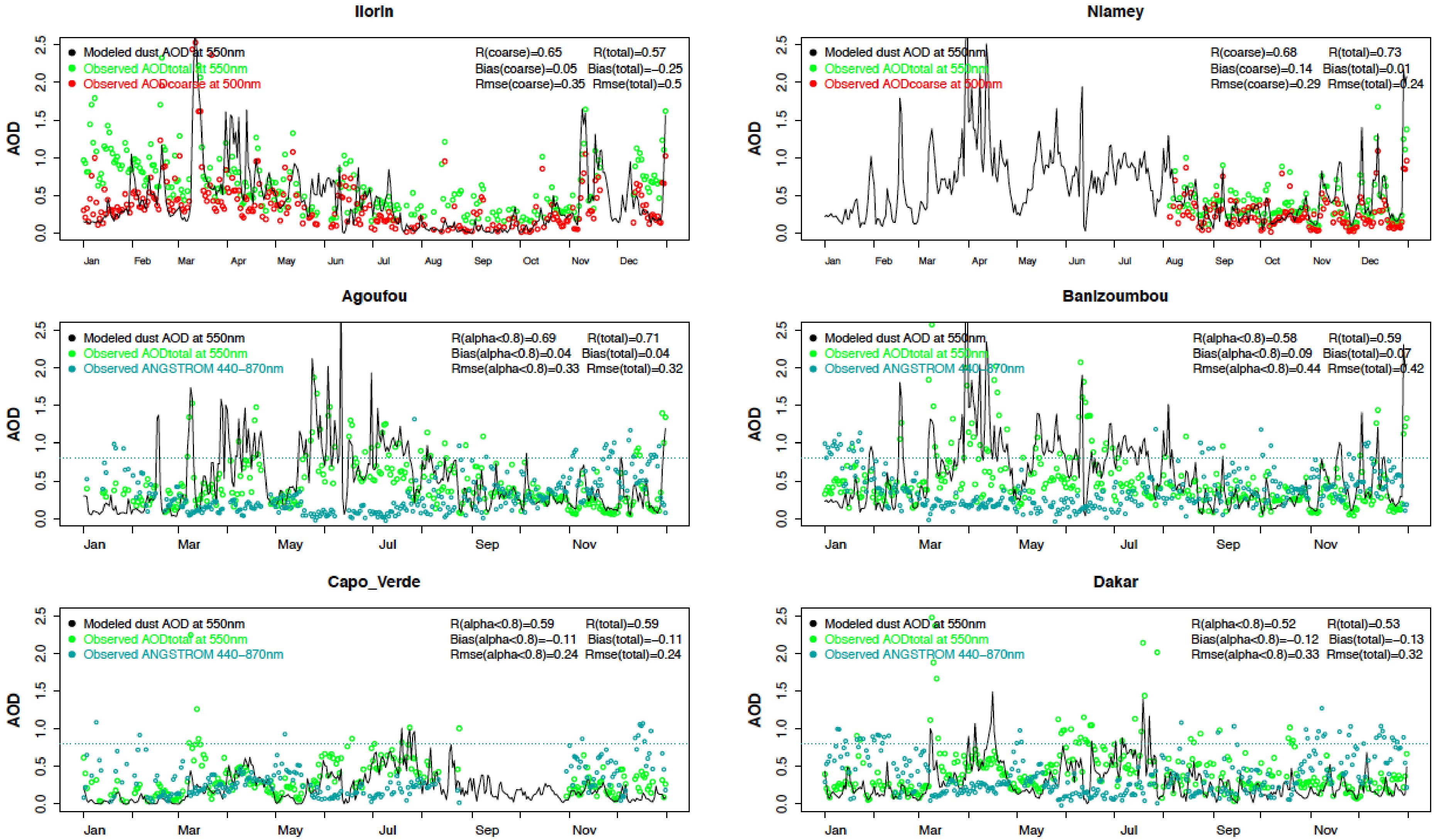
Pérez et al., 2011; Haustein et al., 2012



Pérez et al., 2011 – ACP

Aerosol optical depth on an annual cycle

utación



Pérez et al., 2011 – ACP

Aerosol optical depth near emission sources

Results: Gas-phase chemistry

- Model setup:

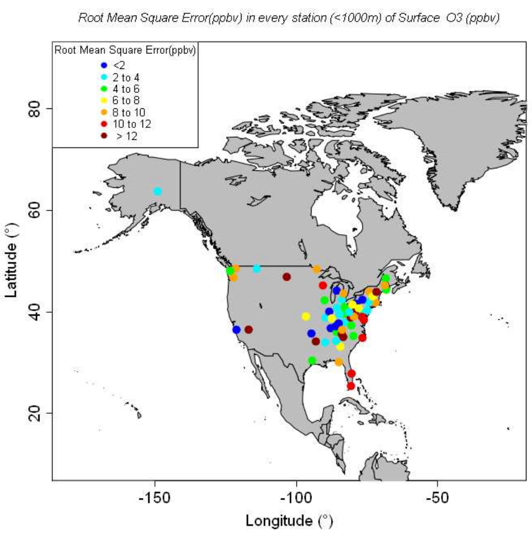
→ Global domain
→ Non-hydrostatic physics
→ 1.4º x 1º horizontal resolution
→ 64 vertical (sigma-hybrid) layers
→ 1º x 1º NCEP/FNL analysis for meteorological initial conditions
→ Chemistry initial conditions from LMDz-INCA
→ Anthropogenic emissions: MOZART 2004
→ Biogenic emissions: MEGAN online model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

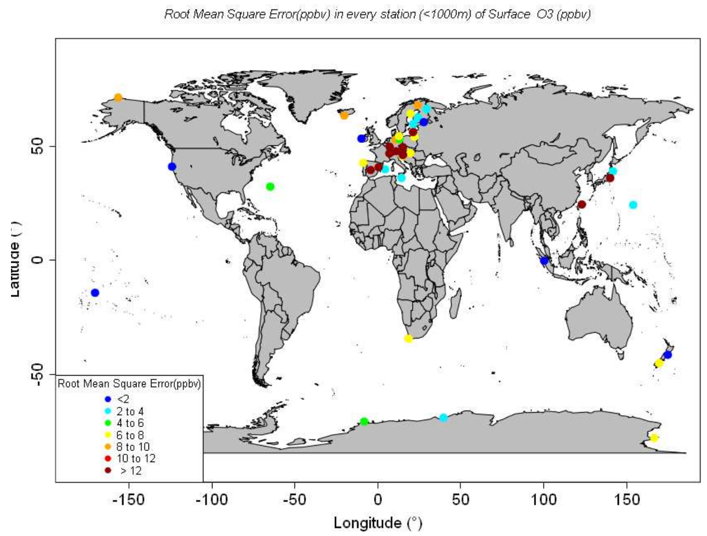
→ Regional domain
→ Non-hydrostatic physics
→ 12km x 12km
→ 24 vertical layers
→ Anthropogenic emissions: EMEP 2004
→ Biogenic emissions: MEGAN online model
→ BC from global run
→ August 2004 simulation

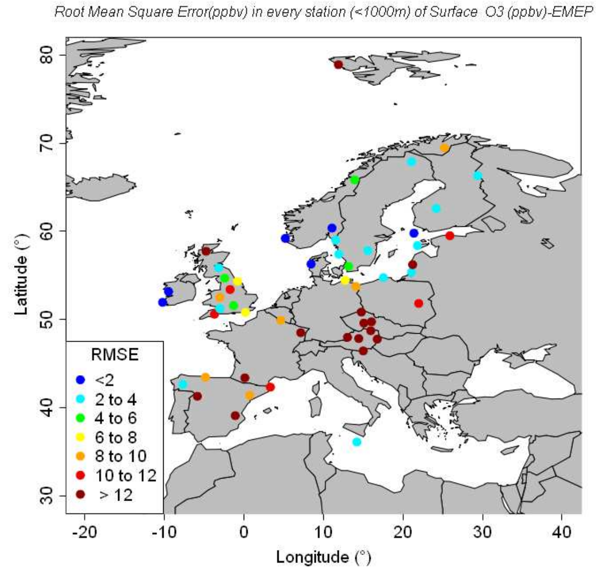
→ All results are preliminary!

Preliminary evaluation with surface and ozonesondes

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



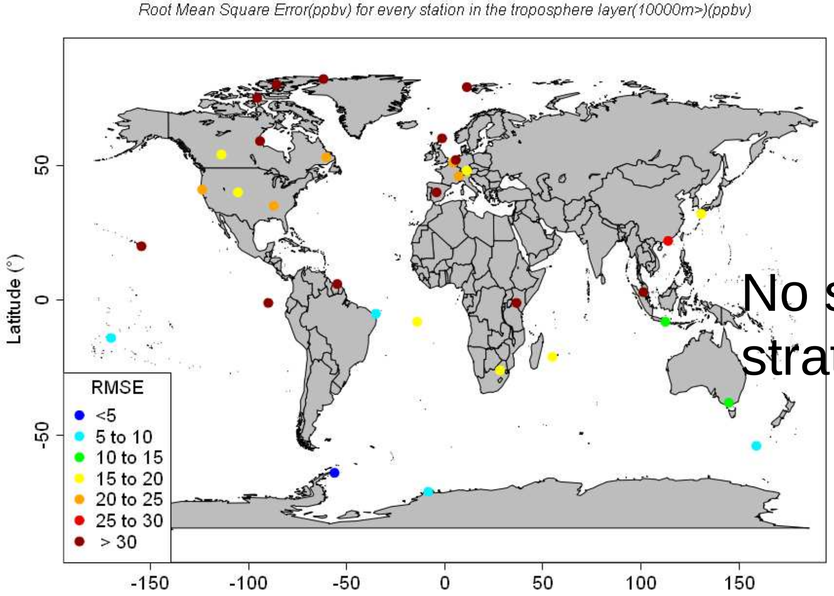




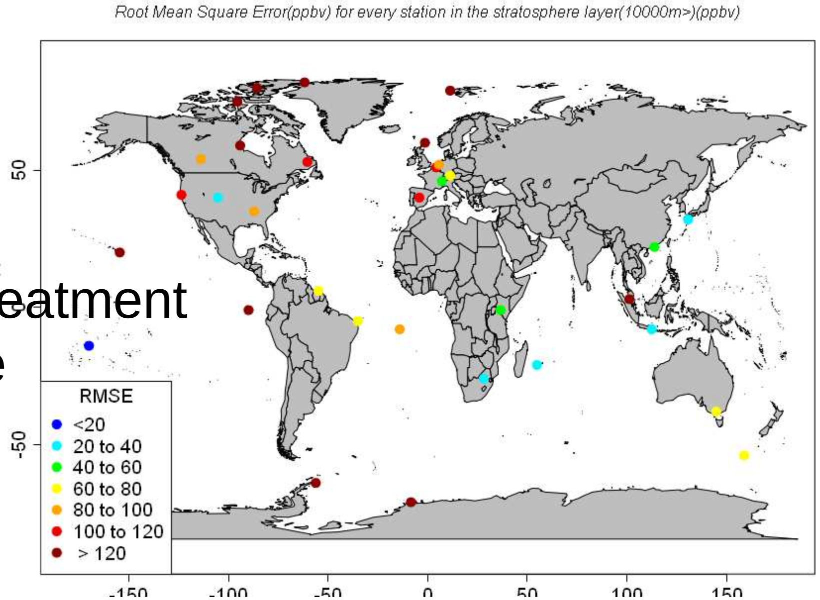
GAS	Mean mod (ppbv)	Mean obs (ppbv)	NDATA	cor	Std (mod)	Std (obs)	RMSE (ppbv)	MB (ppbv)	MAE (ppbv)	MNBE (%)	MNGE (%)
O3 WDCGG	35.149	31.236	1243	0.27	12.7	8.8	13.4	-1	9.9	-0.2	24
O3 EMEP	35.96	34.354	1882	0.27	13.8	8.4	14.1	-1.7	11	-2.5	26.9
O3 CASTNET	38.755	31.959	1848	0.19	11.9	9.4	13.8	1.9	10.7	7.7	26
NO2 EMEP	5.692	4.236	563	0.44	7	4.9	6.7	1.6	4.2	42.5	75.3
CO WDCGG	177.194	122.963	791	0.32	93.3	54	107.6	56.4	67.8	75.9	81.5

RMSE (monthly data) OZONOSONDES (WOULD, CMD and SHADOZ)

TROPO

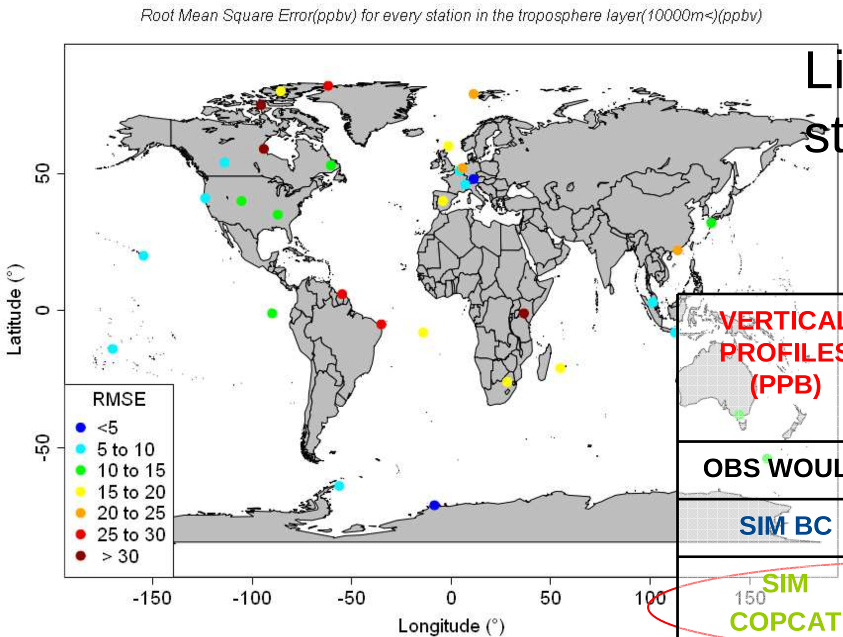


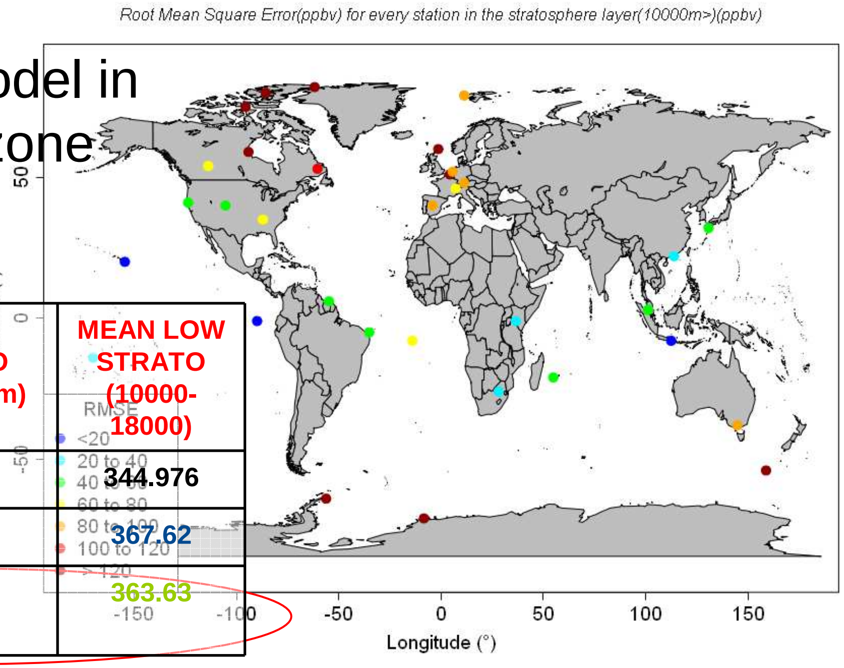
lower STRATO



No specific treatment strato. Ozone

Linear model in strato. Ozone



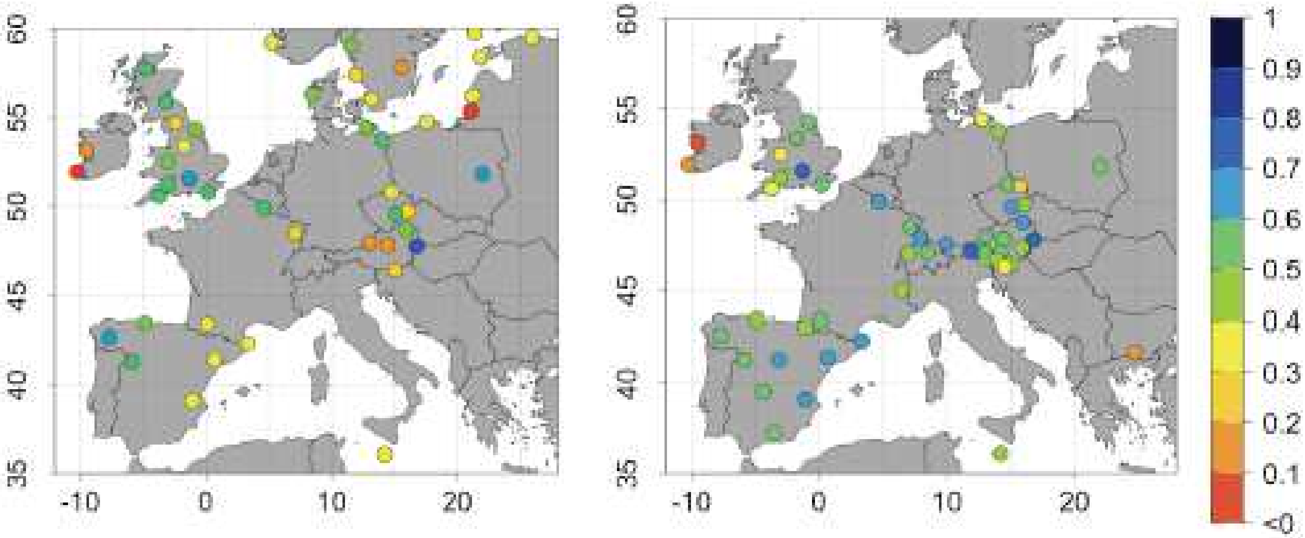


VERTICAL PROFILES (PPB)	MEAN TROPO (<10000m)	MEAN LOW STRATO (10000-18000)
OBS WOULD	50.89	344.976
SIM BC	32.98	367.62
SIM COPCAT	43.42	363.63

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

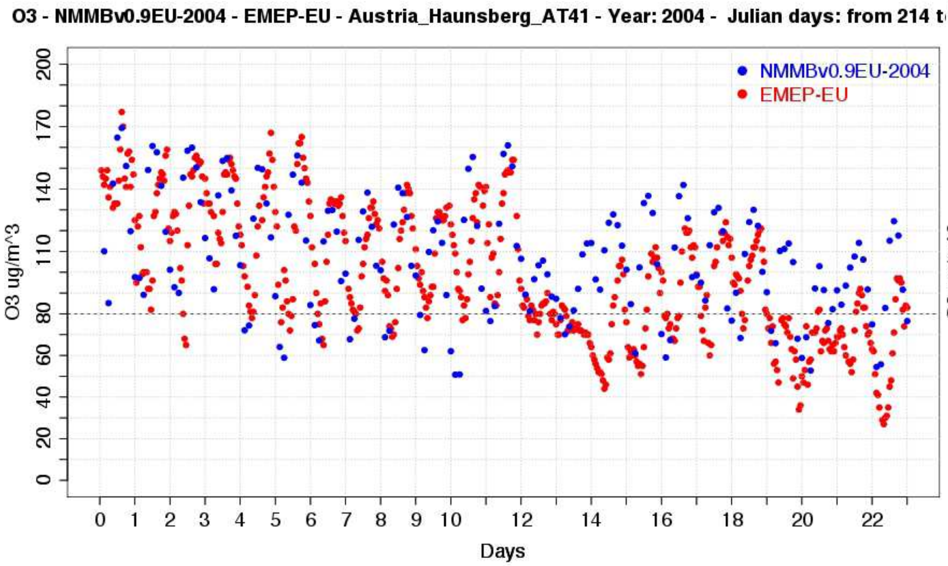
Results for August months for global and regional runs – EMEP background stations

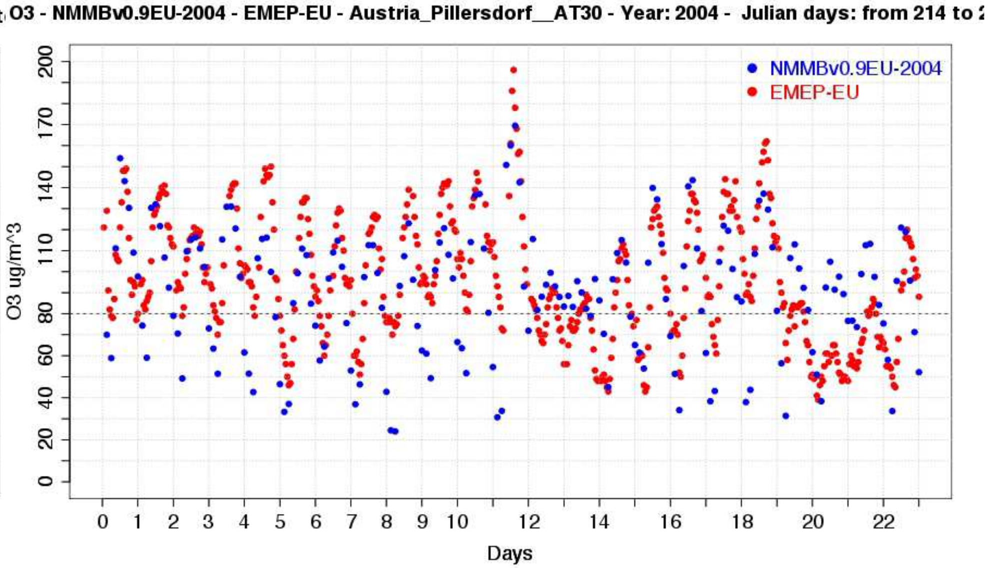
Run	Corr.	MB ($\mu g/m^3$)	RMSE ($\mu g/m^3$)	MNBE (%)	MNGE (%)	MFB (%)	MFE (%)
Global	0.33	-12.9	41.4	-11.5	30.9	-21.3	36.7
Regional	0.51	0.7	23.1	2.1	17.2	-0.3	17.1

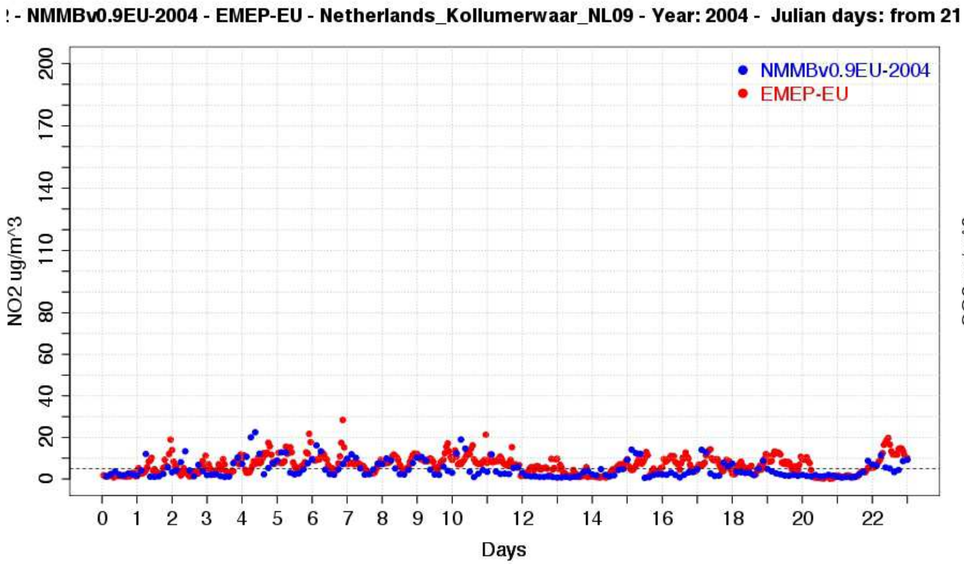


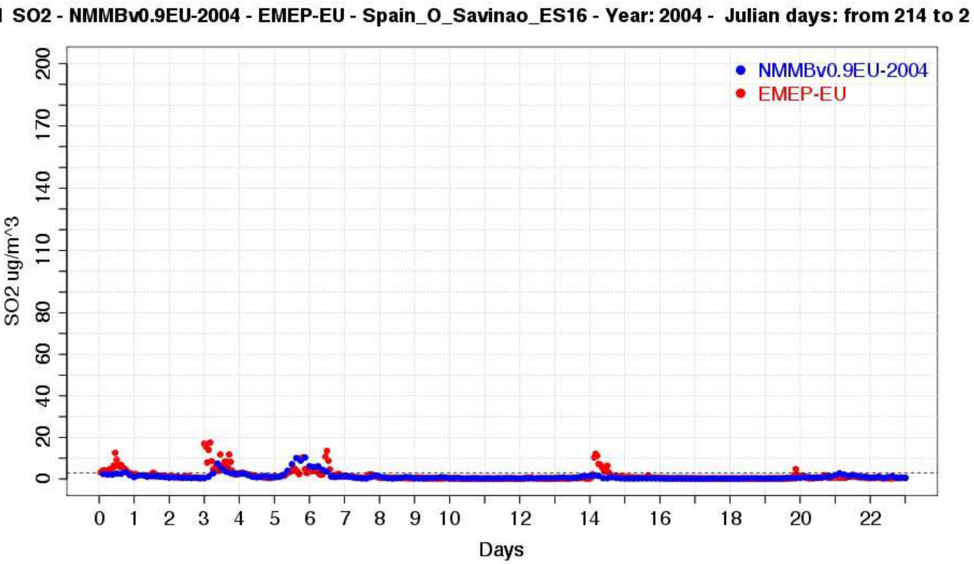
Surface ozone correlation at several EMEP stations – Global (left) and Regional (right)

Regional run: Model vs Obs

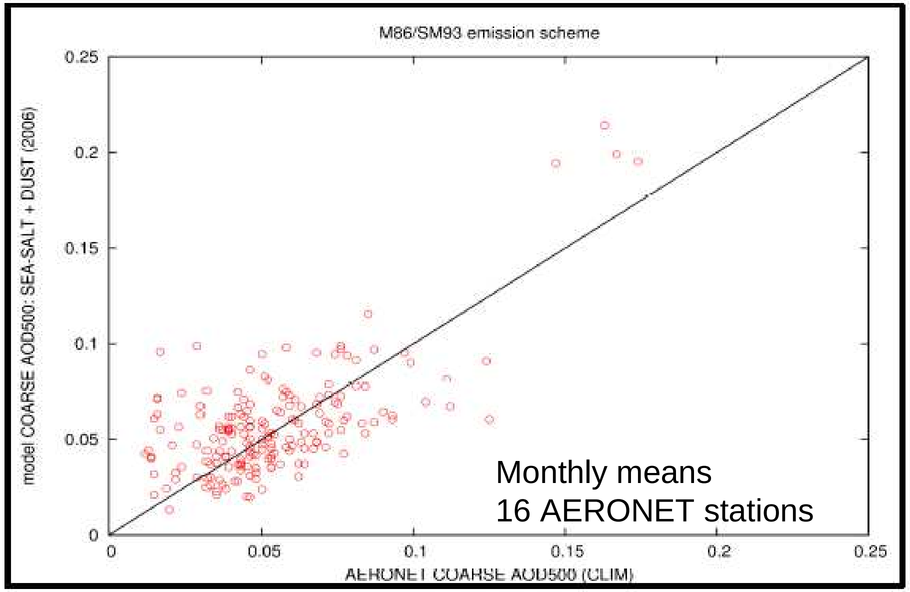


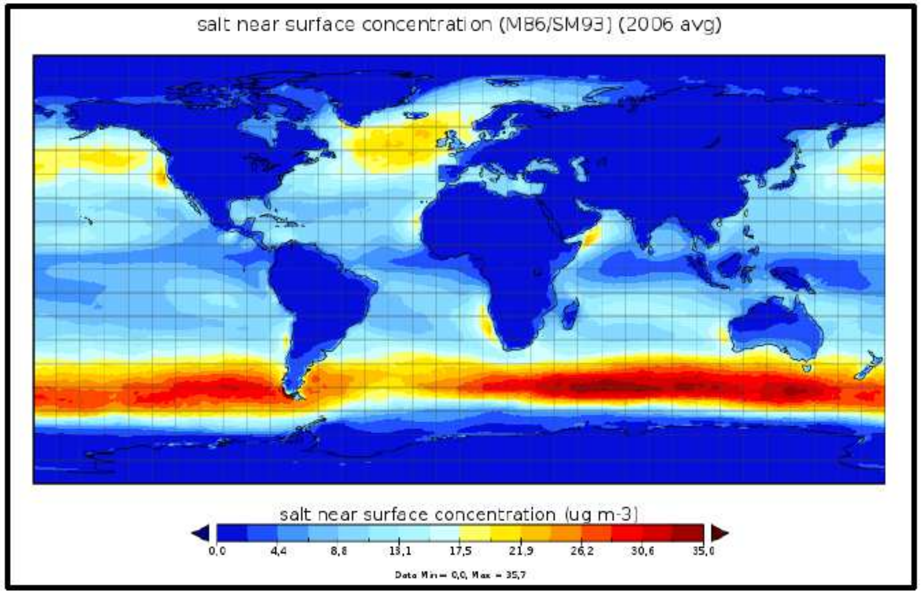


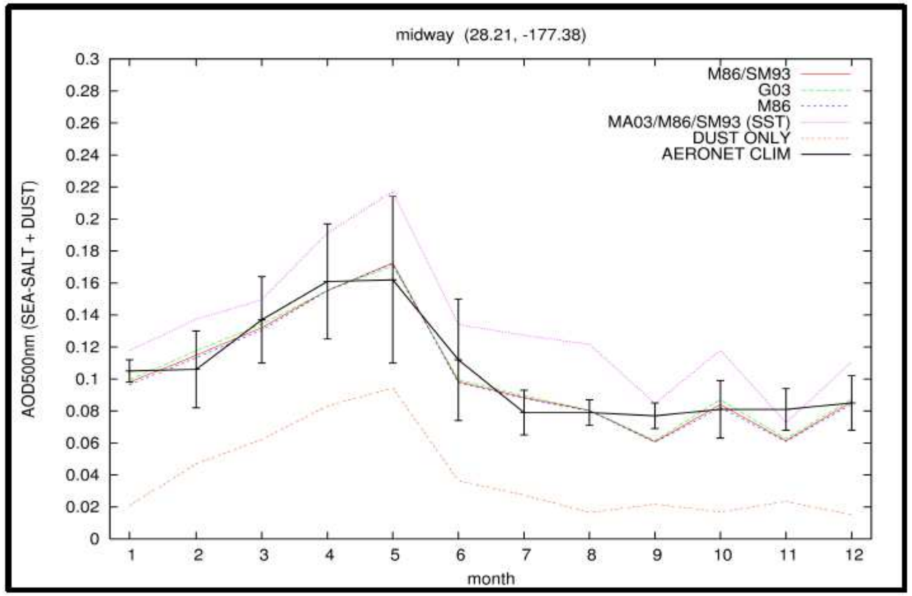


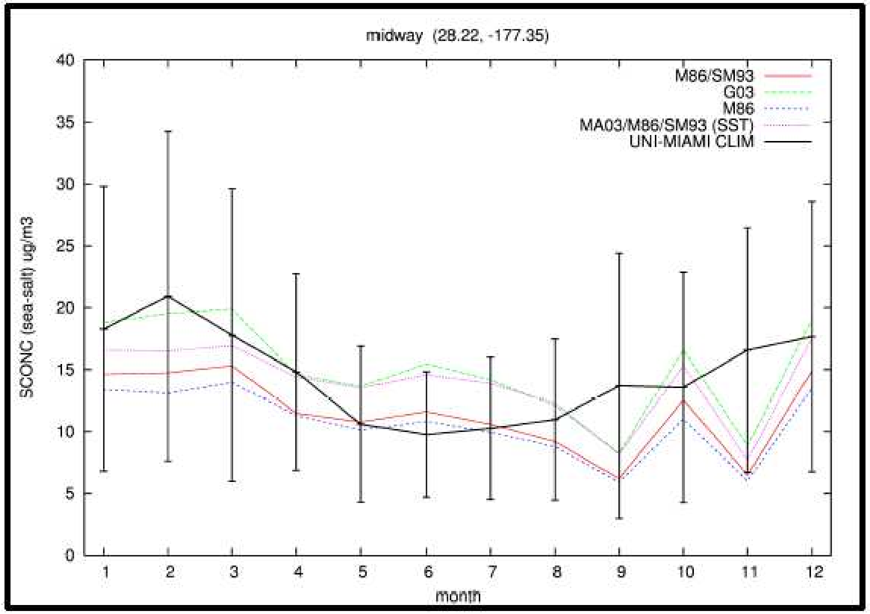


Sea Salt results (Spada et al., 2012) – Global run 2006 at 1ºx1.4º - AOD



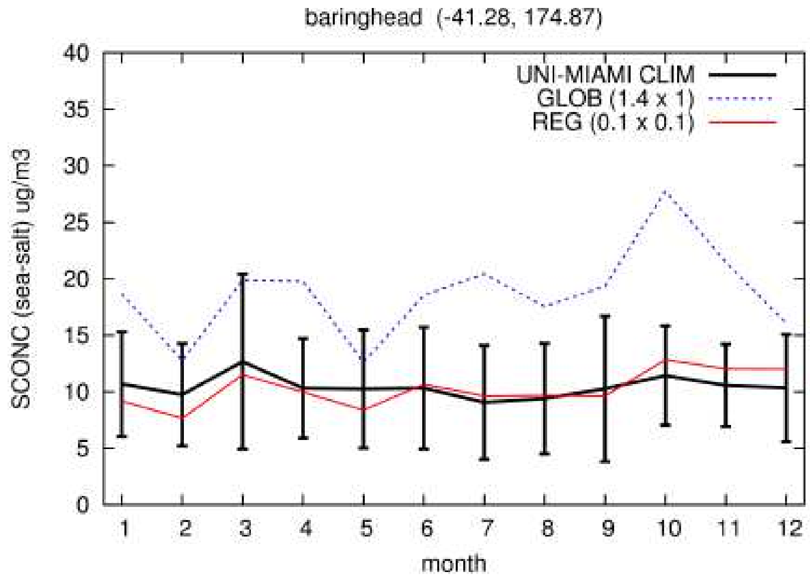


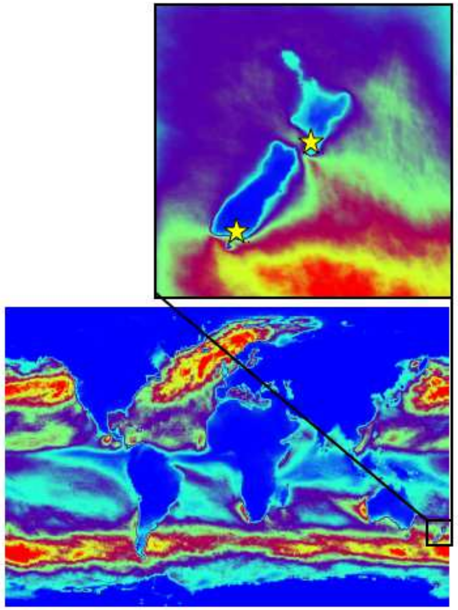




NMMB/BSC-CTM sea-salt: multiscale simulation

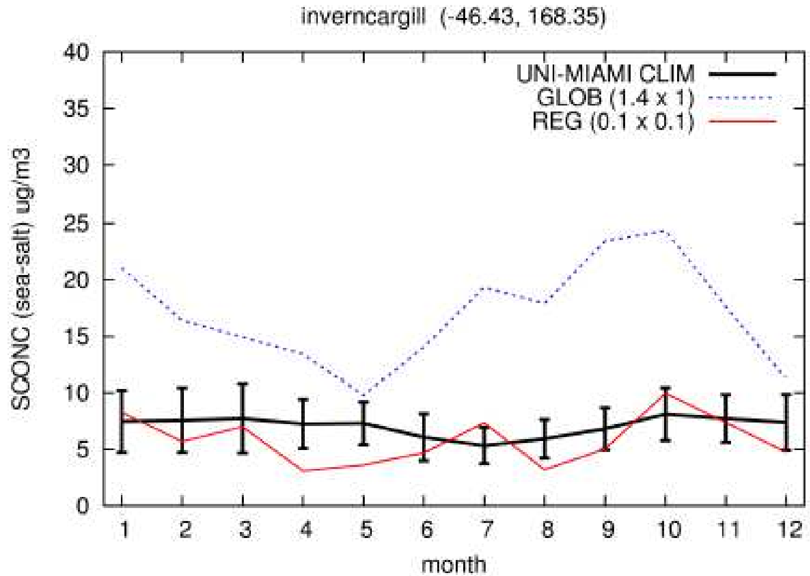
- Same emission scheme
- Consistent physics from global to regional
- Fully on-line aerosol coupling
- Modeled sea-salt concentrations is coastal areas may be strongly affected by resolution
- Global – to – regional: increased capability to resolve both SSA deposition scales and meso circulations





REG:
0.1 x 0.1 deg

GLOB:
1.4 x 1 deg



- Future developments

Future developments (I/II)

- Improvement and evaluation of the chemistry part of the model.
- Implementation of the other global relevant aerosol species, i.e. black (BC) and organic carbon (OC), and sulfate (SO4), in addition to dust (DU) and sea salt (SS).

- It is planned to couple the radiative scheme with all the considered aerosol species to simulate the direct aerosol radiative effect.
- It is planned to couple the model ozone prediction with the radiative scheme of NMMB.
- It is panned to couple the photolysis scheme with the model clouds, ozone, and aerosol species (DU, SS, BC, OC, SO4).

Future developments (II/II)

- Implementation of secondary aerosol schemes (SIA, new SOA parameterizations) for LAM applications at high-resolutions

- Evaluation of the gas-phase chemistry on regional domains

- Experimental dust forecasts on global and regional domains within the SDS-WAS system

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THANK YOU FOR YOUR ATTENTION

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