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Supercomputing
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Centro Nacional de Supercomputación



Atmospheric Chemistry with the online multiscale NMMB-MONARCHv1.0 model: global-regional evaluations and data assimilation capability

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27-29/11/2017

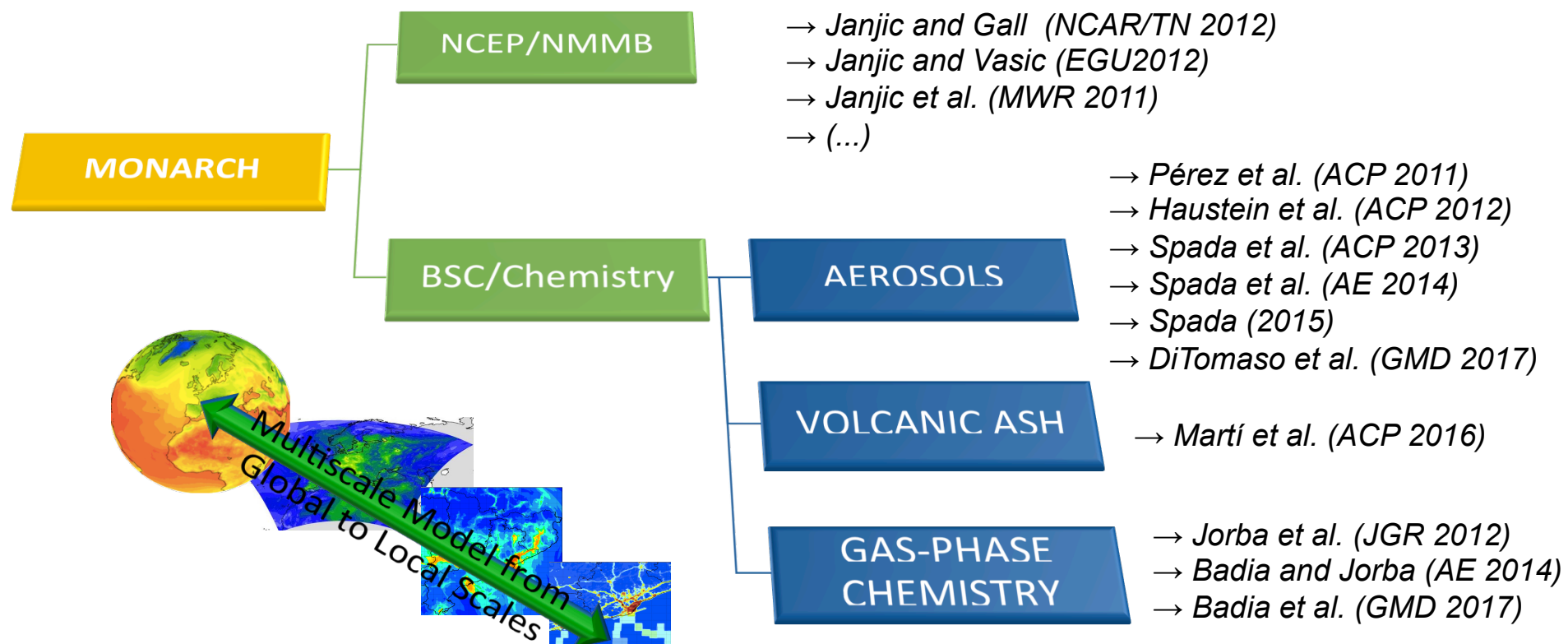
26th GLOREAM meeting

Multiscale: global to regional scales allowed (nesting capabilities)

Non-hydrostatic dynamical core: single digit kilometre resolution allowed

On-line coupling: weather-chemistry feedback processes allowed

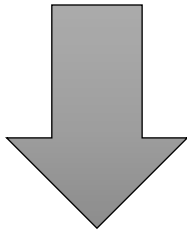
Ensemble-based data assimilation system for aerosols





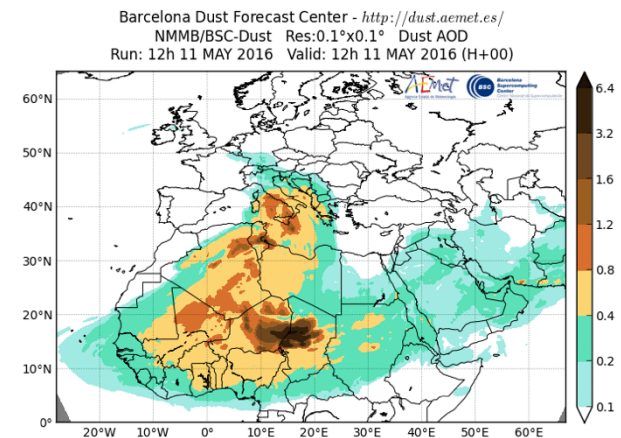
SDS-WAS. North Africa, Middle East and Europe Regional Center - *Research*
Started in 2010

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



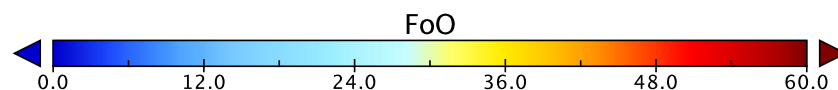
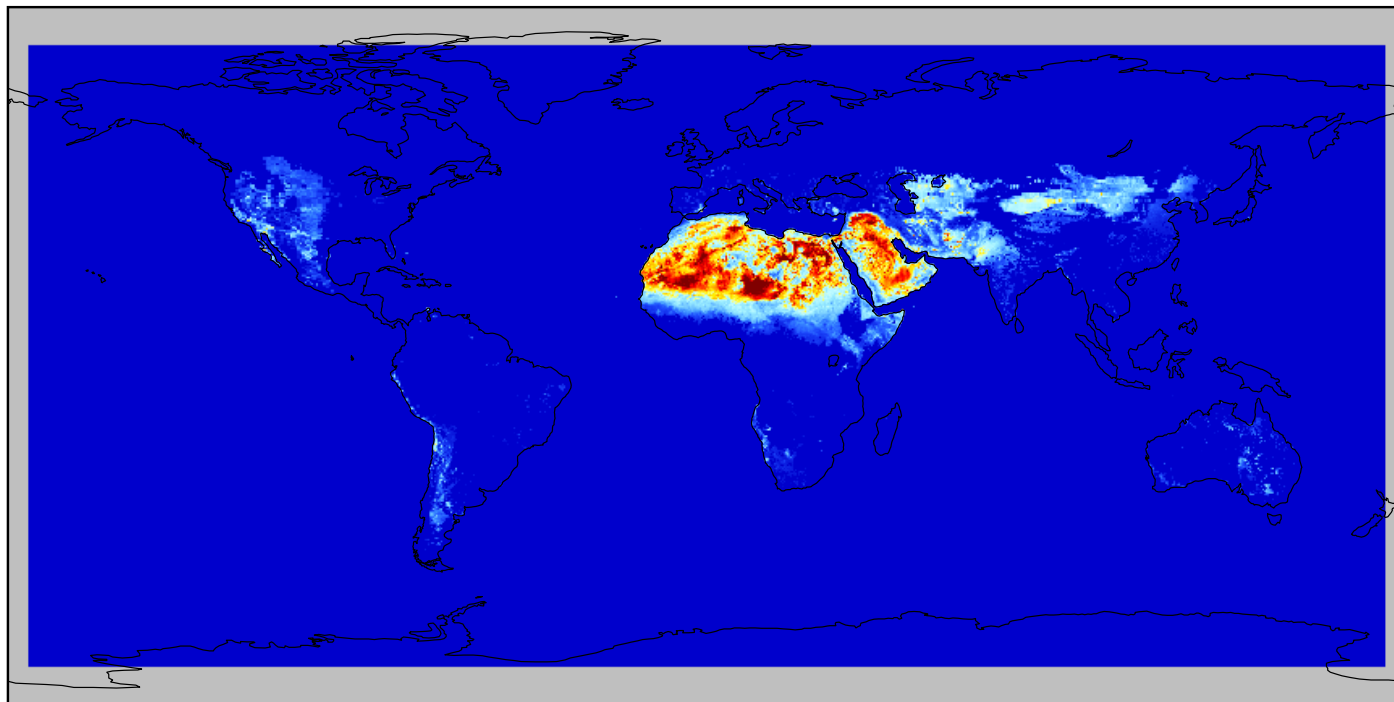
Barcelona Dust Forecast Center - *Operations*
First specialized WMO Center for mineral dust prediction. Started in 2014

<http://dust.aemet.es>  [@Dust_Barcelona](https://twitter.com/Dust_Barcelona)

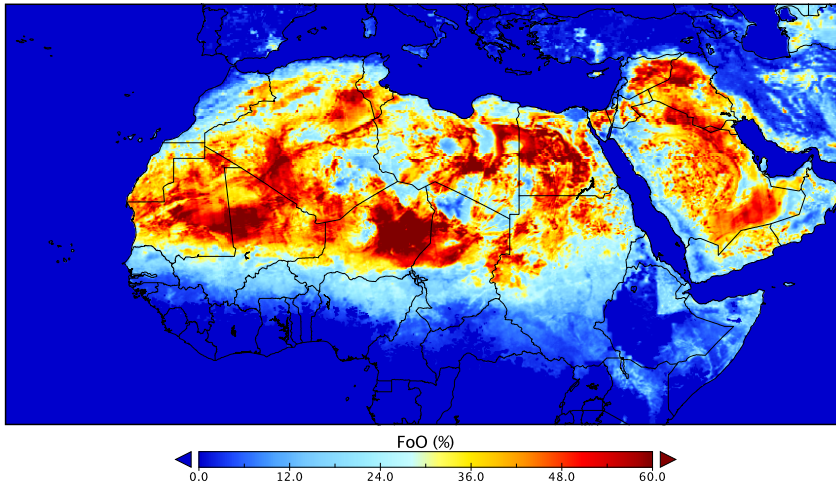


- Sea-salt: Jaeglé et al. (2011) wind and sst
- Dust: source location based on MODIS DB, vertical flux scaled with the topographic source of Ginoux - 2001

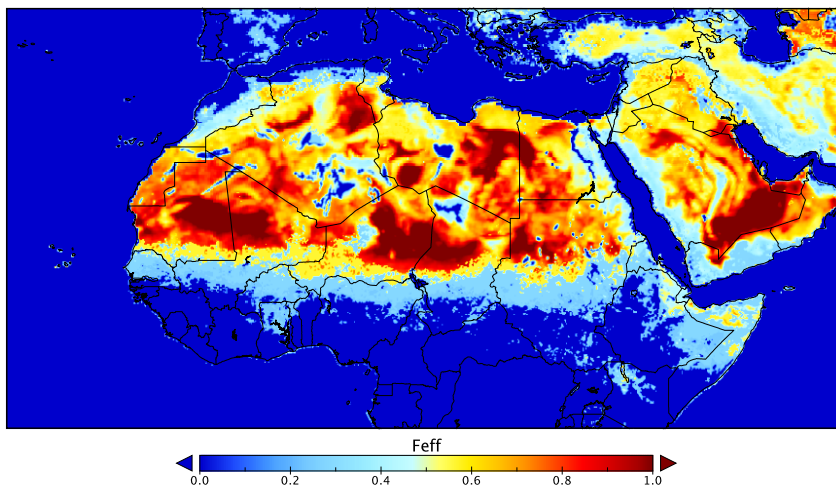
Frequency of Occurrence DoD > 0.2



Frequency of Occurrence DoD > 0.2



Feff in drag partition



- 3 emission schemes with drag partition:
 - NMMB original (~Maticorena based scheme)
 - GOCART scheme
 - New Kok scheme (Kok et al., 2014)

$$U^* t = \frac{U^* t_s}{f_{eff}} \quad f_{eff} = 1 - \frac{\ln(z_0/z_{0s})}{\ln(0.7(X/z_{0s})^{0.8})}$$

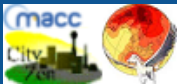
z_0 based on satellite static roughness +
monthly vegetation (LAI) from MODIS

A multiscale emission modeling framework

- A **stand-alone tool** for simulating **emissions** on a **user-defined grid** for **global, regional and urban** air quality models.
- Users can **select, combine and scale multiple inventories** through a flexible configuration file to obtain **hourly gridded emissions**.

Emission data library

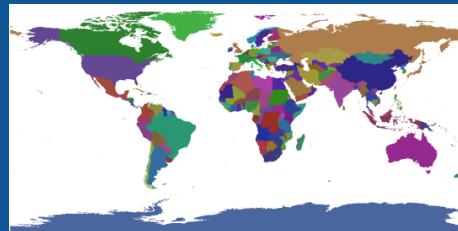
- Multiple **global and regional emission inventories**
- **Online emissions:**
 - Biogenic (MEGAN), lightning, ocean
- Spanish bottom-up emission inventory (street level emissions)



(...)

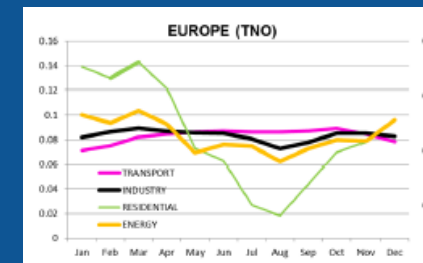
Conservative regridding

- **User-defined grid:**
 - Regular lat-lon
 - Rotated lat-lon
 - LCC
- **Masking and scaling factors to combine and update emission inventories**



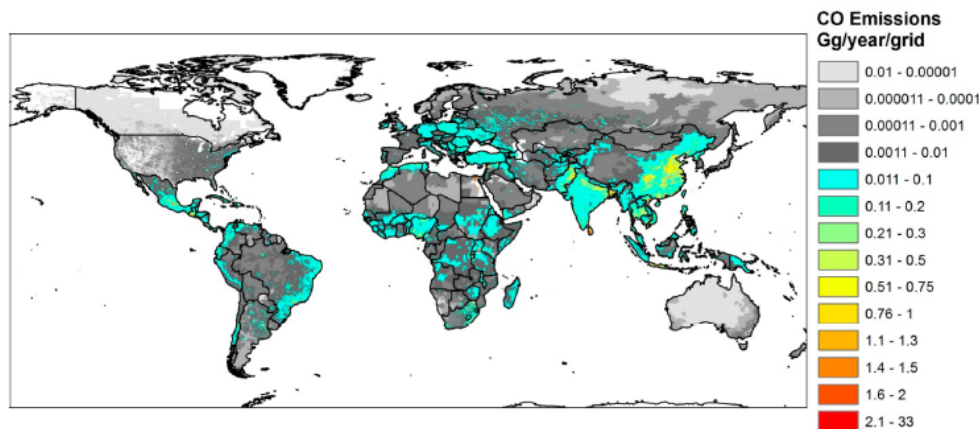
Vertical, temporal, speciation

- **Vertical profiles:**
 - Point sources, biomass burning, air traffic
- **Temporal profiles:**
 - Monthly, weekly and daily factors per sector
- **VOC and PM2.5 speciation:**
 - CB05, SAPRC99, AERO5, AERO6



- Residential waste burning emissions** have a significant contribution to **global OC**. These emissions are mainly occurring in **developing and poor countries**

species	open waste burning	total reported anthropogenic	ref
ammonia (NH ₃)	1.1 Tg	47 Tg	HTAP v2 for 2008 ^c
sulfur dioxide (SO ₂)	486 Gg	109 Tg	HTAP v2 for 2008 ^c
nitrogen oxides (NO _x as NO)	3.6 Tg	113 Tg	HTAP v2 for 2008 ^c
PM _{2.5}	10 Tg	34 Tg	HTAP v2 for 2008 ^c
PM ₁₀	12 Tg	51 Tg	HTAP v2 for 2008 ^c
BC	632 Gg	5.5 Tg	HTAP v2 for 2008 ^c
OC	5.1 Tg	12 Tg	HTAP v2 for 2008^c

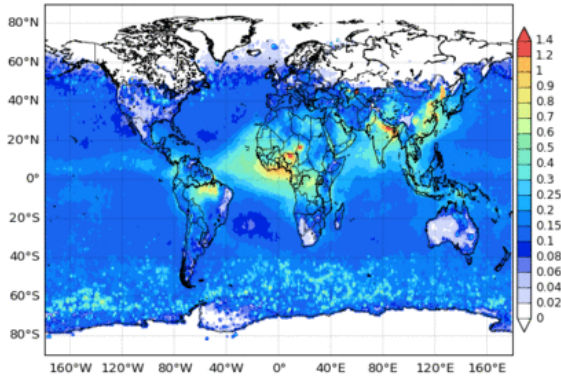


Wiedinmyer et al. (2014)

**For this sector, PM_{2.5}-BC-OC accounts for 42.7% of total PM_{2.5}.
All PM_{2.5}-BC-OC is considered PM_{FINE}**

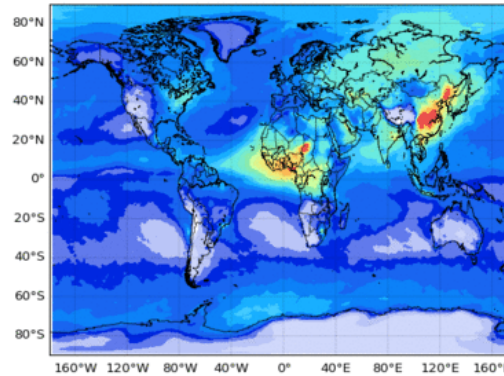
MODIS C6 Level 3

MODIS/Terra-Aqua AOD550 Collection 6 Level 3
2015 DJF



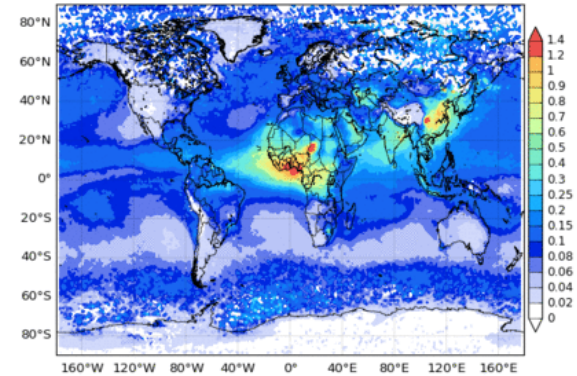
MONARCH All Sky

NMMB-MONARCH-b015 AOD550
2015 DJF



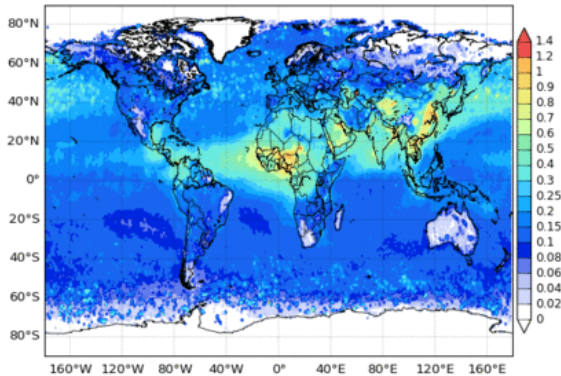
MONARCH Clear Sky

NMMB-MONARCH-b015 AOD550
2015 DJF

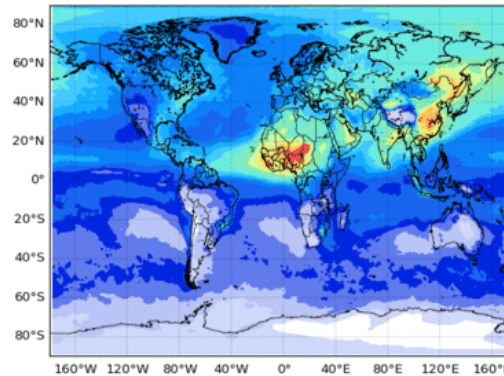


DJF

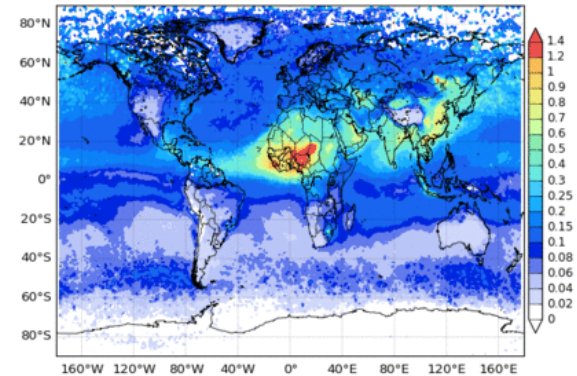
MODIS/Terra-Aqua AOD550 Collection 6 Level 3
2015 MAM



NMMB-MONARCH-b015 AOD550
2015 MAM



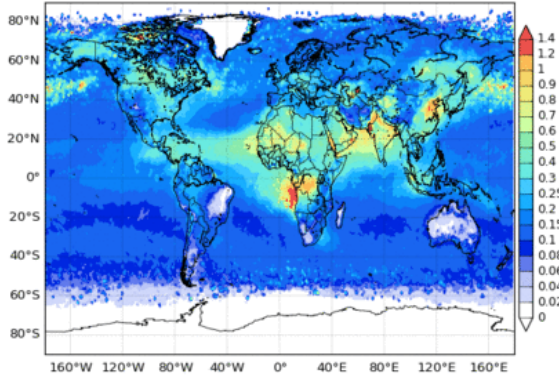
NMMB-MONARCH-b015 AOD550
2015 MAM



MAM

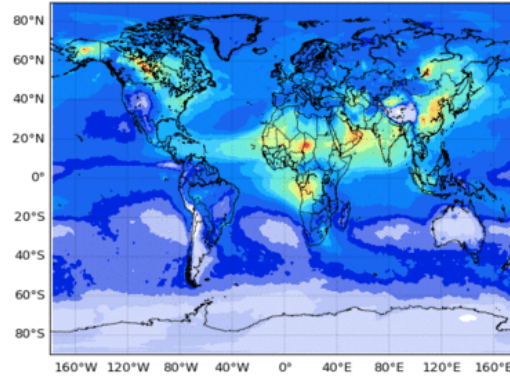
MODIS C6 Level 3

MODIS/Terra-Aqua AOD550 Collection 6 Level 3
2015 JJA



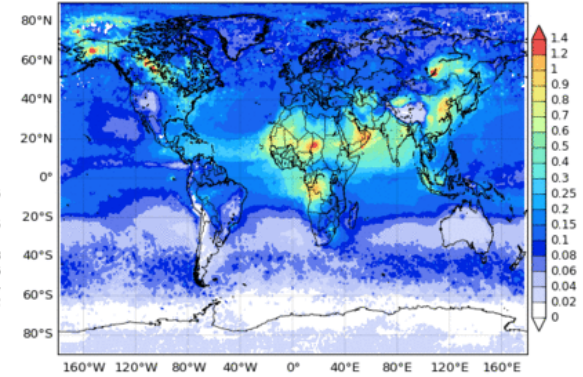
MONARCH All Sky

NMMB-MONARCH-b015 AOD550
2015 JJA



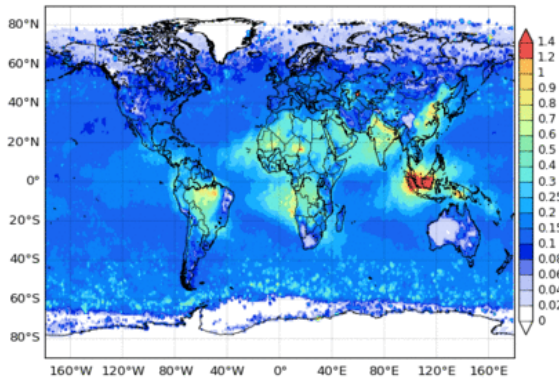
MONARCH Clear Sky

NMMB-MONARCH-b015 AOD550
2015 JJA

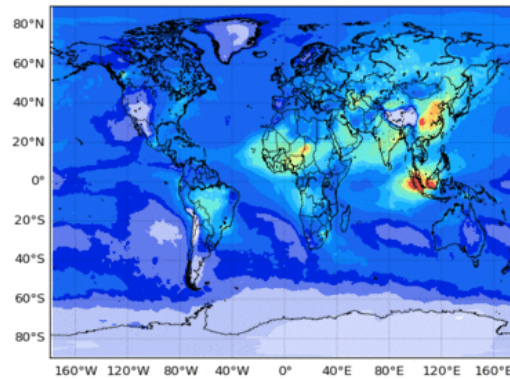


JJA

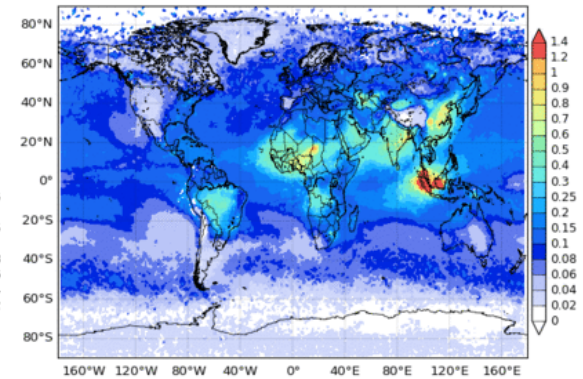
MODIS/Terra-Aqua AOD550 Collection 6 Level 3
2015 SON



NMMB-MONARCH-b015 AOD550
2015 SON

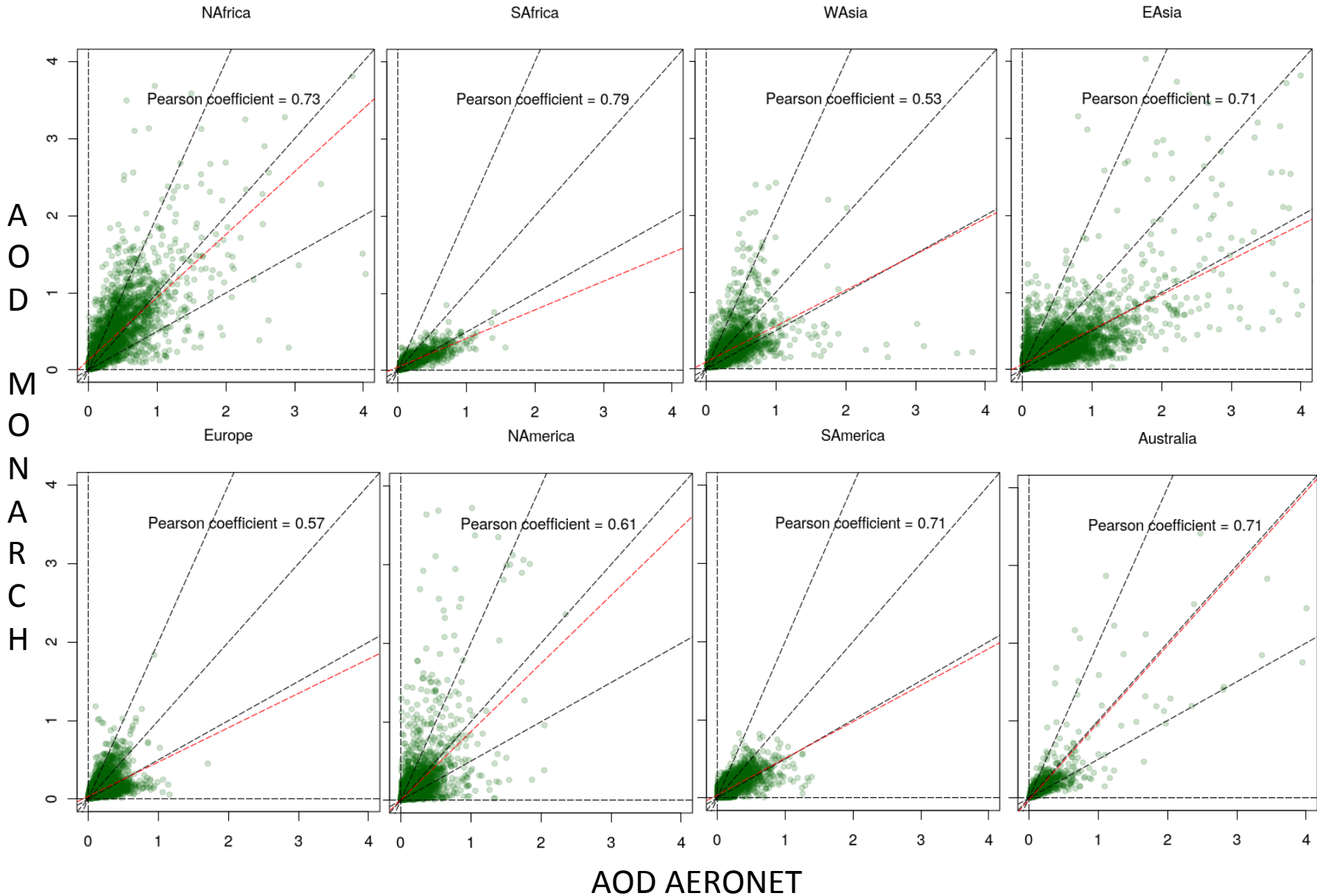


NMMB-MONARCH-b015 AOD550
2015 SON

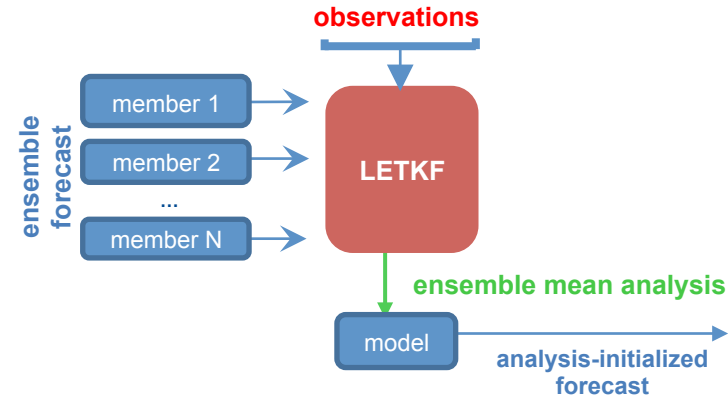


SON

AOD Evaluation 2015



NMMB-MONARCH coupled with a Local Ensemble Transform Kalman Filter (**LETKF**) for the assimilation of aerosol optical depth observations

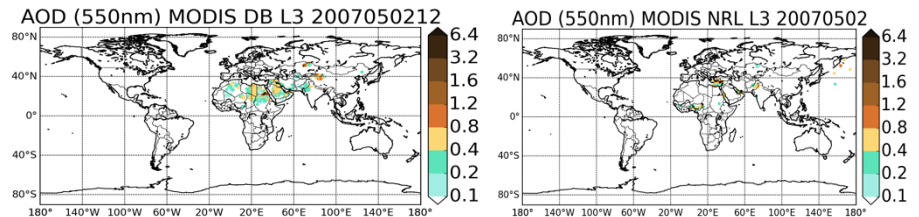


Mineral dust application

The ensemble forecast is based on uncertainties in the dust emission scheme

- vertical flux,
- size distribution at emission
- threshold on friction velocity

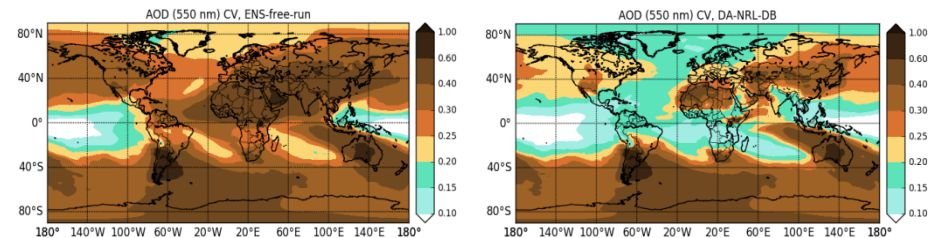
Assimilated satellite observations, filtered for dust



MODIS Deep Blue

MODIS Dark Target

Ensemble spread reduction where obs are present



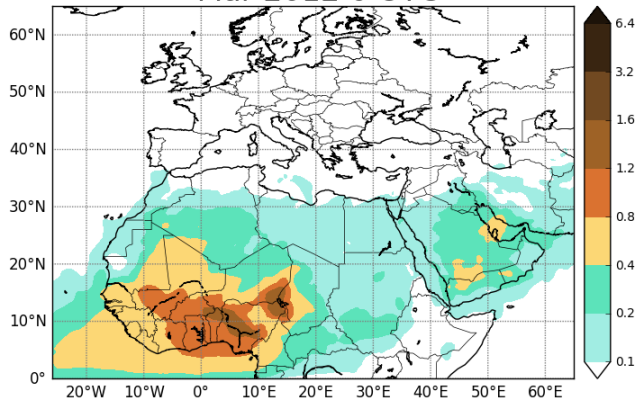
Ensemble free run

DA run

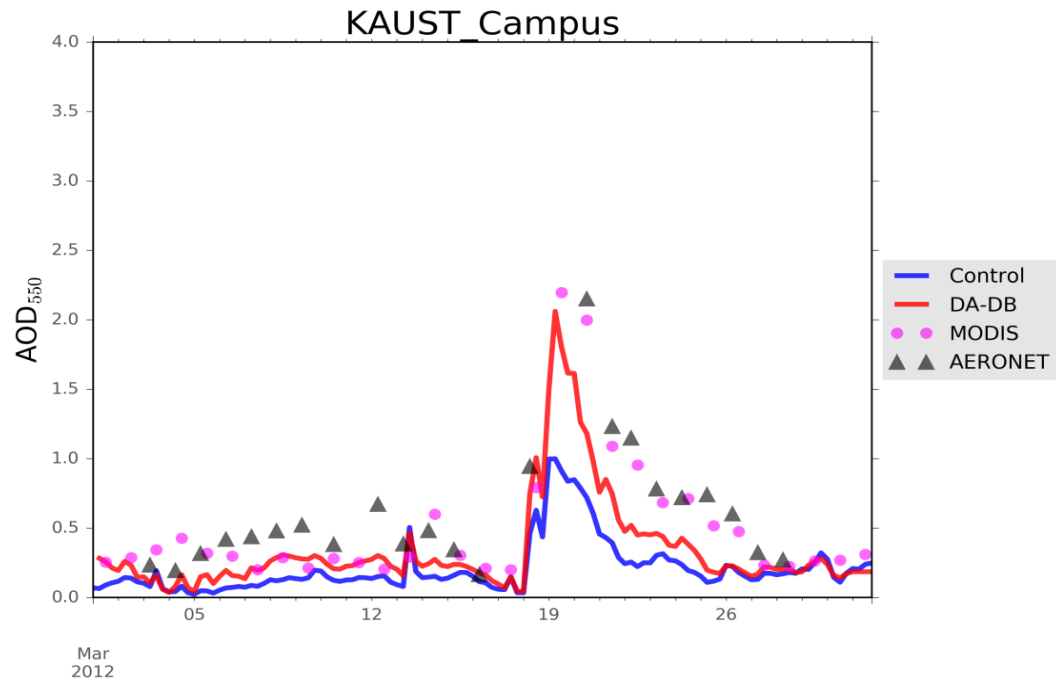
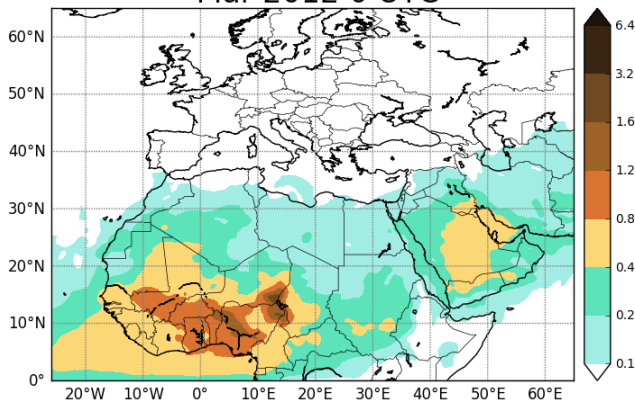
Assimilation of 0.1x0.1 deg MODIS Deep Blue coarse DOD based on Ginoux et al., 2012

First assimilation tests with
MONARCH at 0.3x0.3 deg resolution

Dust AOD (550nm), control
Mar 2012 0 UTC

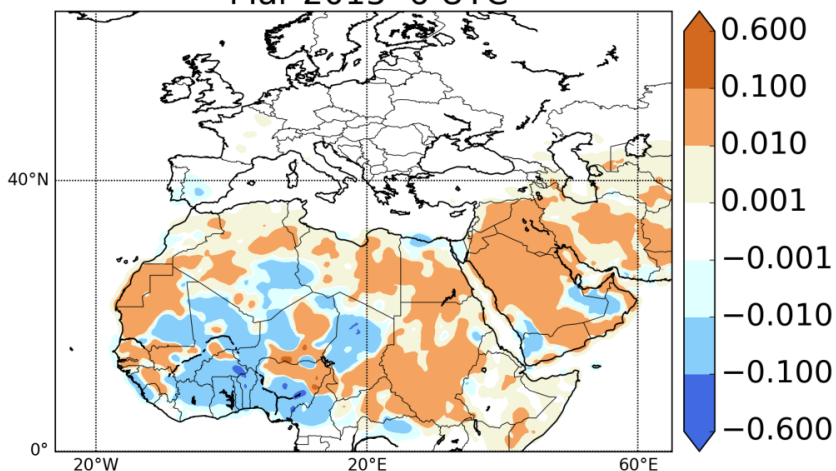


Dust AOD (550nm), analysis
Mar 2012 0 UTC

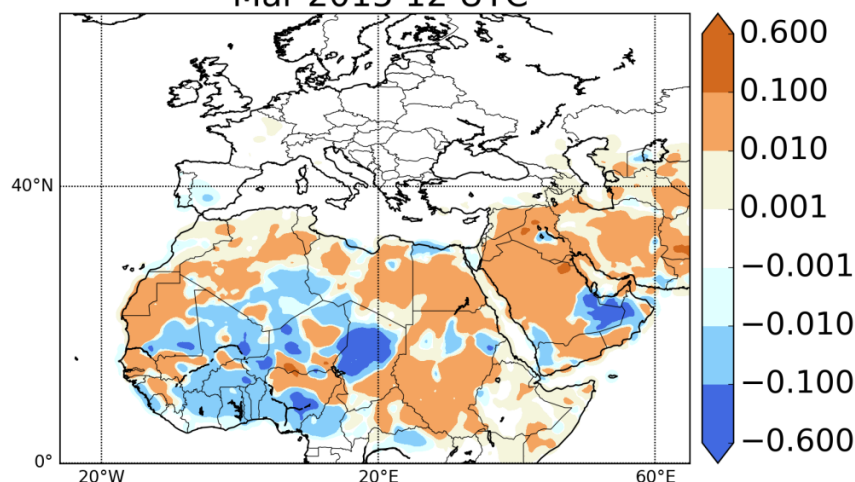


Feedback from assimilation increments

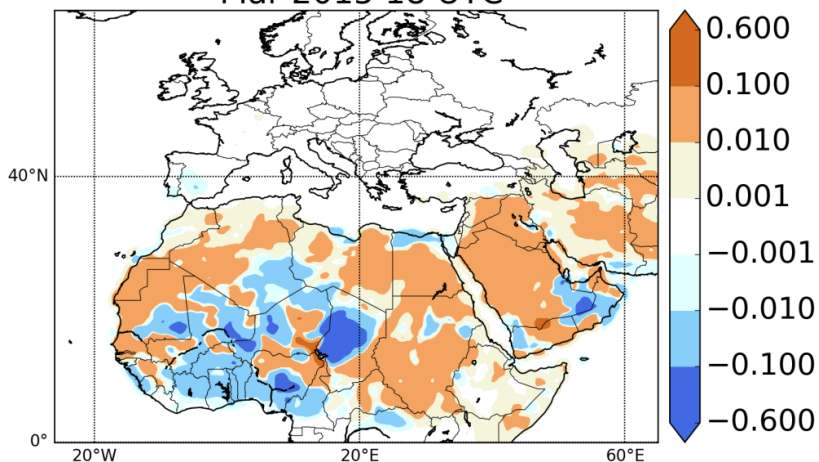
Dust AOD (550nm) analysis - first guess
Mar 2015 6 UTC



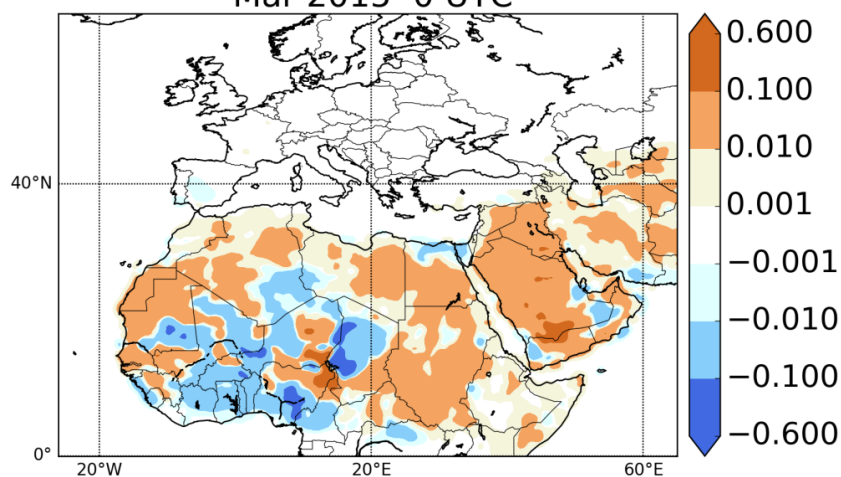
Dust AOD (550nm) analysis - first guess
Mar 2015 12 UTC



Dust AOD (550nm) analysis - first guess
Mar 2015 18 UTC

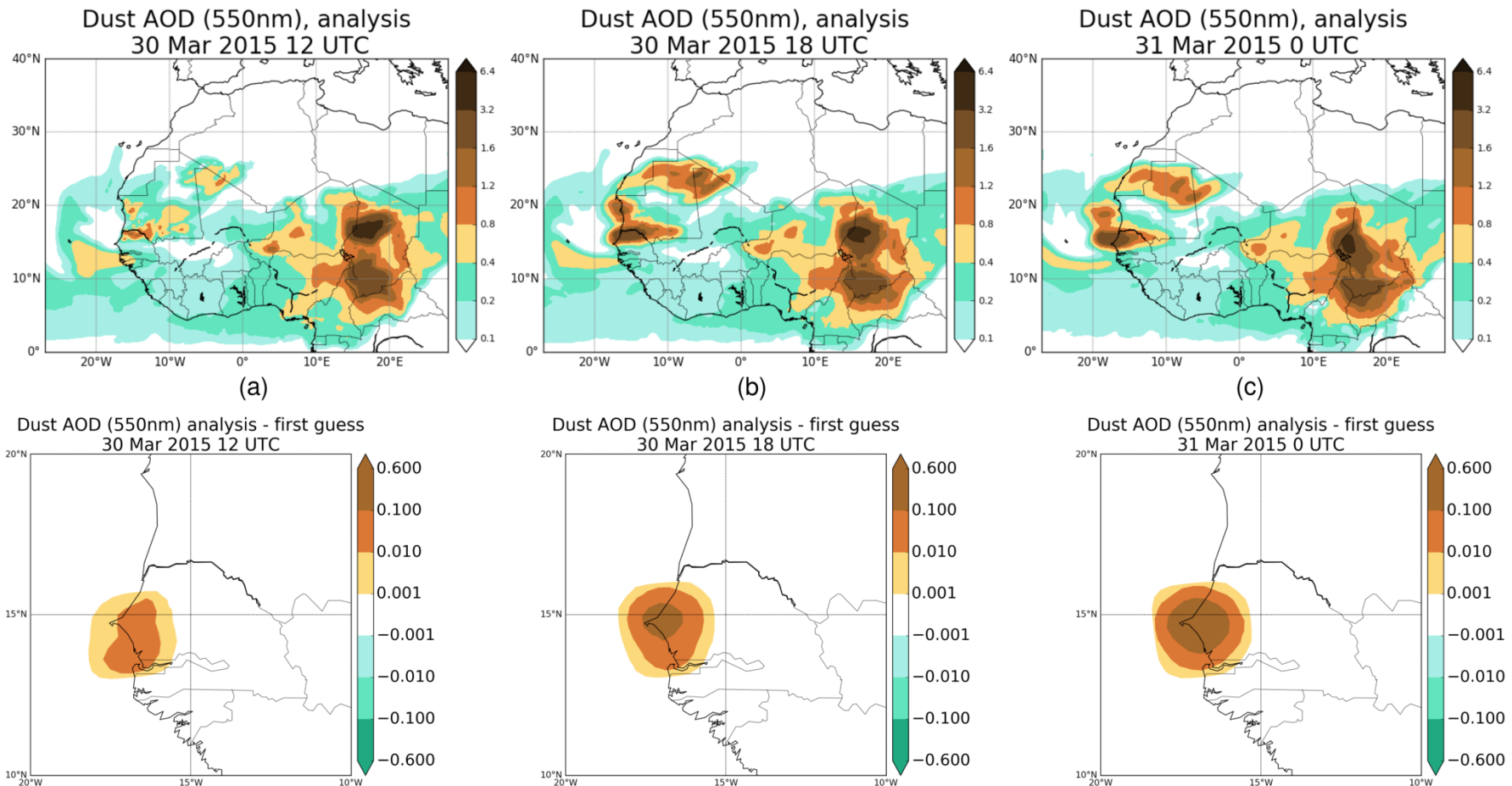


Dust AOD (550nm) analysis - first guess
Mar 2015 0 UTC



Evaluating the potential of ACTRIS-2 data for assimilation through pilot dust case studies

Multi-wavelength Mie-Raman lidar profile observations provided by the University of Lille for the M'bour site outside Dakar

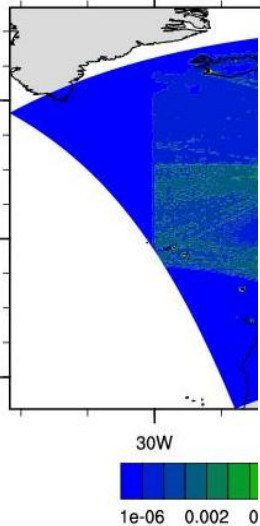


Regional run results (Badia and Jorba, 2014; Ulas et al., 2014)



NMMB/BSC-CTM 20100701 12 UTC - AQMEII2 domain

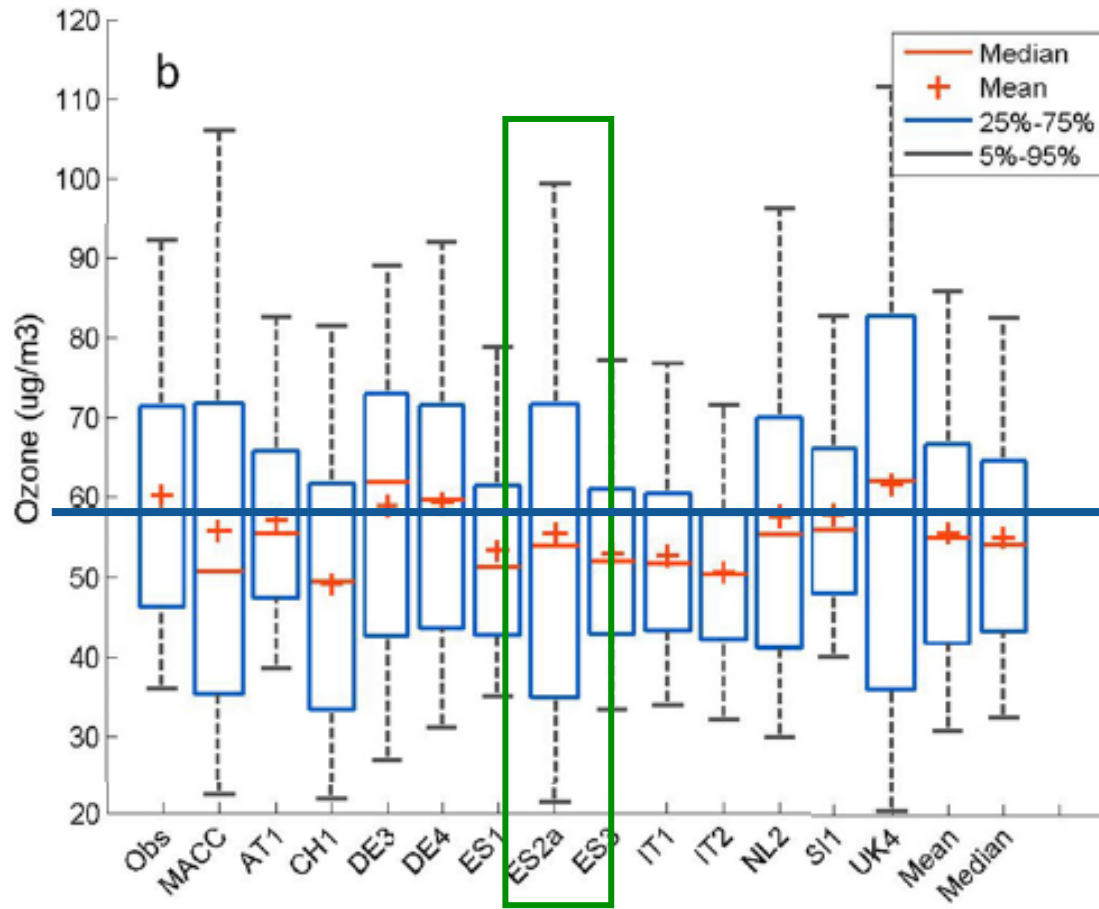
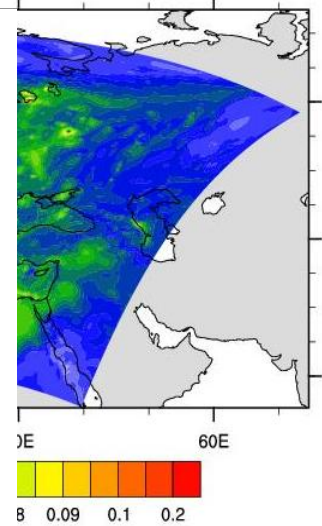
total column NO2 emissions



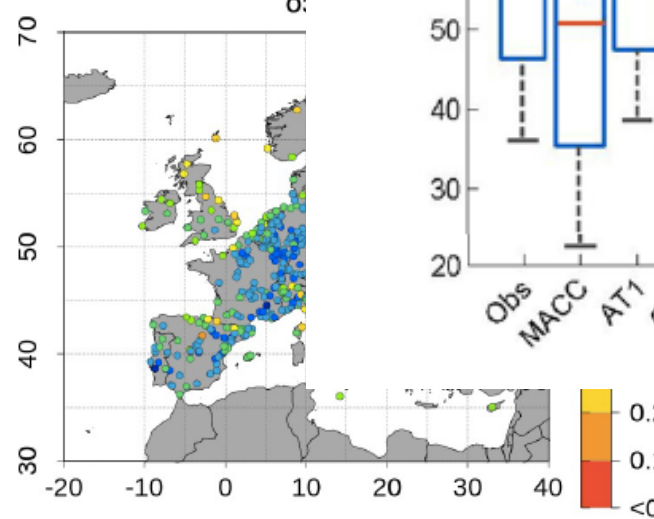
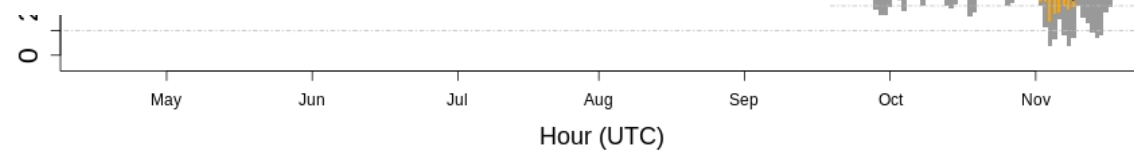
NMMB/BSC-CTM 20100715 12 UTC - AQMEII2 domain

O3 -UMO

ppmv



ISE=20.2 MB=-2.2



CURRENT FORECASTING – DEVELOPED/AVAILABLE – UNDER DEVELOPMENT - PLANNED

DOMAIN	GLOBAL (ICAP)	REGIONAL North Africa, Middle East and Europe (SDS-WAS)	REGIONAL Europe/Iberian Peninsula/Urban Areas (CALIOPE)
Model	MONARCH	MONARCH	CMAQ (DREAM for dust) MONARCH
Status	QO	O	O
Meteorology	Inline: NMMB	Inline: NMMB	Offline: WRF-ARW Inline: NMMB nesting
Resolution	1.4x1 deg 0.7x0.5 deg	0.1x0.1 deg 0.03x0.03 deg	0.1x0.1 / 0.04x0.04 / 0.01 x0.01
levels	24 48	40 60-70	30 60-70
DA	LETKF	LETKF	NA LETKF
Assimilated Obs	MODIS DT+DB (DU) MODIS DT+DB (ALL)	MODIS DT+DB (DU)	NA MODIS DT+DB (ALL)
Aerosol Species	DU, SS, BC , POA , SOA bio, SOA anthro , SU, NI	DU	CMAQ (AERO5) MONARCH aerosols
Gas phase chemistry	CBM-IV CB05 ONLINE and CLIMATOLOGY		CB05 CB05
Emissions	HERMES 3.0 (HTAP v2) MEGAN ONLINE		EMEP, MEGAN / HERMES, MEGAN/ HERMES MEGAN
Bio. Burn. Emissions	GFAS NRT		NA NRT



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Thank you

Contact: oriol.jorba@bsc.es

Chemical mechanism

CBM-IV and CB05 KPP implementation, and CB05 EBI solver.

Rate constants updated based on evaluations of Atkinson et al., (2004) and Sander et al., (2006).

Photolysis scheme

On-line Fast-J scheme (Wild et al., 2000).

Coupled with physics of each model layer (e.g., clouds, absorbers as ozone).

The quantum yields and cross sections for the CB05 photolytic reactions have been revised and updated following the recommendations of Atkinson et al., (2004), Sander et al., (2006) and Barnard et al., (2004).

Dry deposition

Wesely et al. (1986, 1989) implemented to compute deposition velocities.

Wet deposition

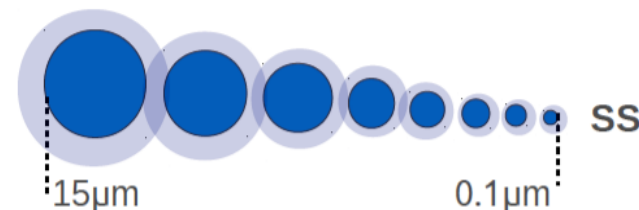
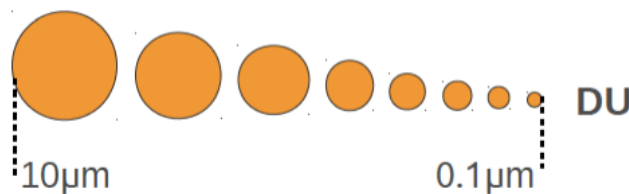
Wet deposition of 36 gases from the CB05 mechanism.

Cloud chemistry includes: scavenging, mixing, wet deposition and aqueous chemistry

Scavenging and wet deposition implemented for gridscale and sub-gridscale clouds following Foley et al. (2010).

Sectional

dust (DU)
sea-salt (SS)



Bulk

Black Carbon (BC)



Organic Aerosols (OA)

Primary Organic Aerosols (POA)

Secondary organic aerosols (SOA)

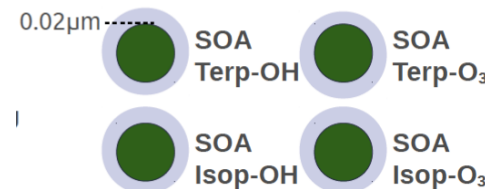
4 gaseous tracers (OH, O₃, TERP, ISOP). Online emission (MEGAN)

4 aerosol-phase hydrophilic tracers

2-product scheme of Tsigaridis and Kanakidou (2007)

Oxidation by OH and O₃ and gas-particle partitioning

Anthropogenic SOA from Toluene and Xylene under development



Sulfate, Nitrate and Ammonium (SU, NI, NH₄)

4 additional prognostic tracers (SO₂, DMS, H₂O₂, H₂SO₄)

3 online or climatological oxidants (OH, O₃, HO₂)

gas-phase oxidation of SO₂, DMS and H₂O₂ by OH

aqueous-phase oxidation by H₂O₂ and O₃

EQSAM Thermodynamic Equilibrium (NH₃, HNO₃, SU+H₂SO₄)



EI	Sector	Year	Pollutants	Vertical	Temporal
GFASv1.2 Kaiser et al. (2012)	Biomass burning	2015	oc, bc ^(*) , so2, pm25,c2h6s	Plume top = Sofiev et al. (2012) Distribution=50 % top 50% uniform below	Daily
HTAPv2.2 Janssens- Maenhout et al. (2015)	energy	2010	oc,bc,so2, pm25,pm10	218-724 m (Bieser et al., 2011)	Monthly
	industry			72-292 m (Bieser et al., 2011)	
	residential			First layer	
	transport			First layer	Yearly (monthly flat profile)
	air_lto			0 – 1 km	
	air_cds			1 – 9 km	
	air_crs			9 – 12 km	
	ships			First layer	
Wiedinmyer et al. (2014)	Residential trash burning			First layer	
MOZART Horowitz et al. (2013)	Ocean	2000	c2h6s	First layer	Monthly

(*) Scaling factors applied: bc → 6.1 and oc → 3.1 (Rémy et al., 2017)