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EXCELENCIA
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BSC UPDATE

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Atmospheric Composition Group

Earth Sciences Department

Barcelona Supercomputing Center

26/06/2017

9th ICAP Meeting, Lille France

Development of MONARCH

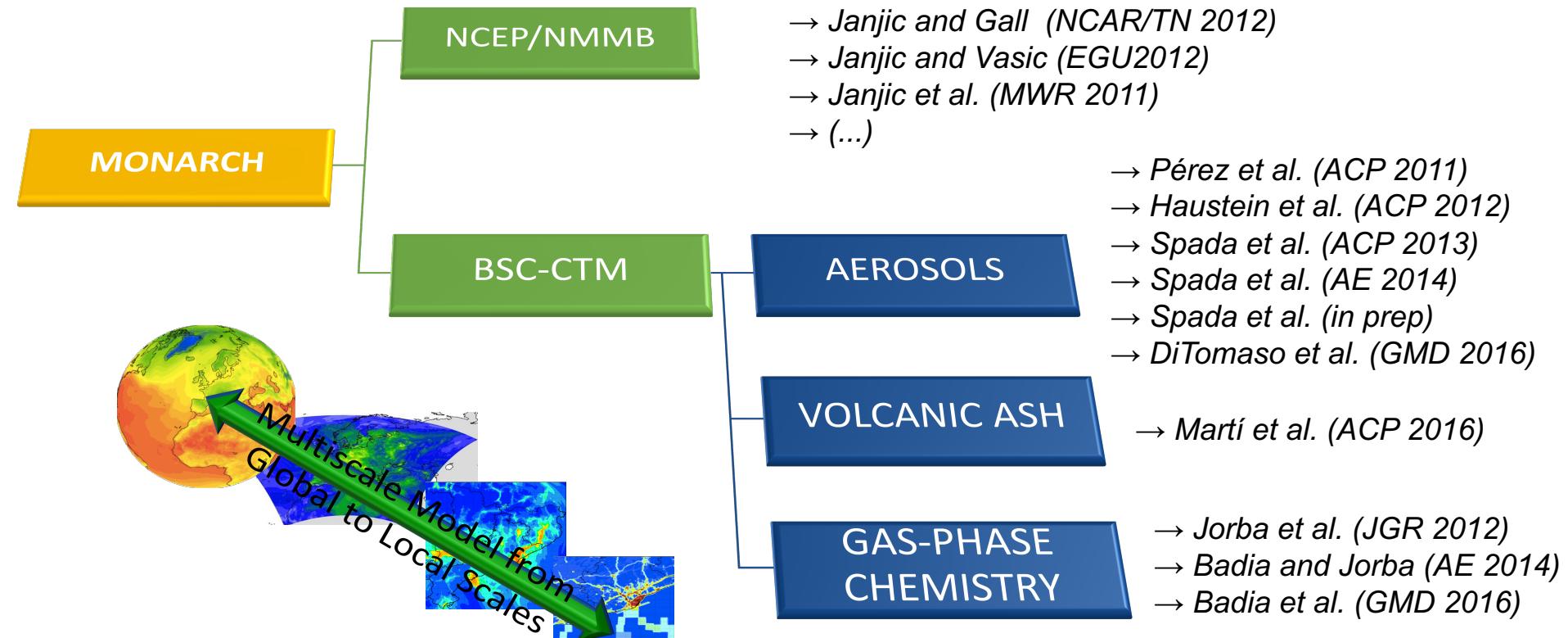
Multiscale Online Non-hydrostatic Atmosphere Re Chemistry model



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- 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



Model features

Physics schemes

- Non-hydrostatic Multiscale Model NMMB
(Janjic et al., 2004)
- Arakawa B grid (Arakawa and Lamb, 1977)
- Vertical hybrid σ -pressure coordinate system
(Simmons and Burridge, 1981)
- A rotated longitude-latitude coordinated system is used for regional simulations
- Radiation: RRTMG
- Convection: Betts-Miller-Janjic (BMJ)
(Betts, 1986)
- Clouds and microphysics: Ferrier (Ferrier et al., 2002)
- Turbulence: Mellor-Yamada-Janjic (MYJ)
(Janjic, 2001)
- Land model: NCEP NOAH (Eck et al., 2003) and LISS

BSC Current forecasts and plans

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

MONARCH: Aerosols



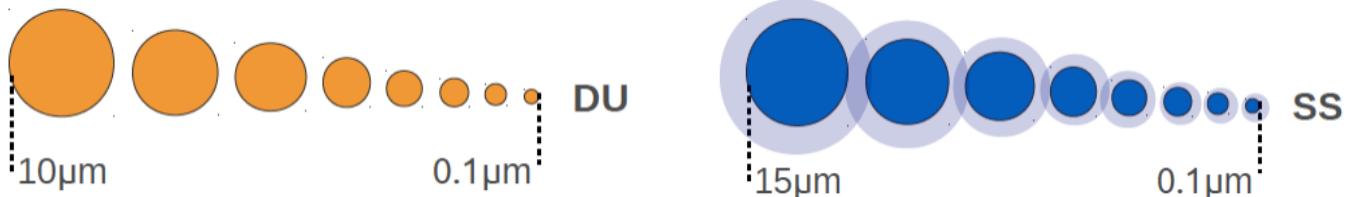
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Sectional

dust (DU)

sea-salt (SS)



Bulk

Black Carbon (BC)



Organic Aerosols (OA)

Primary Organic Aerosols (POA)

Secondary organic aerosols (SOA)

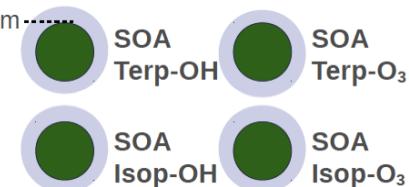
4 gaseous tracers (OH, O₃, TERP, ISOP). Online emission (MEGAN)

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



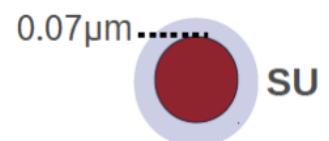
Sulfate (SU):

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

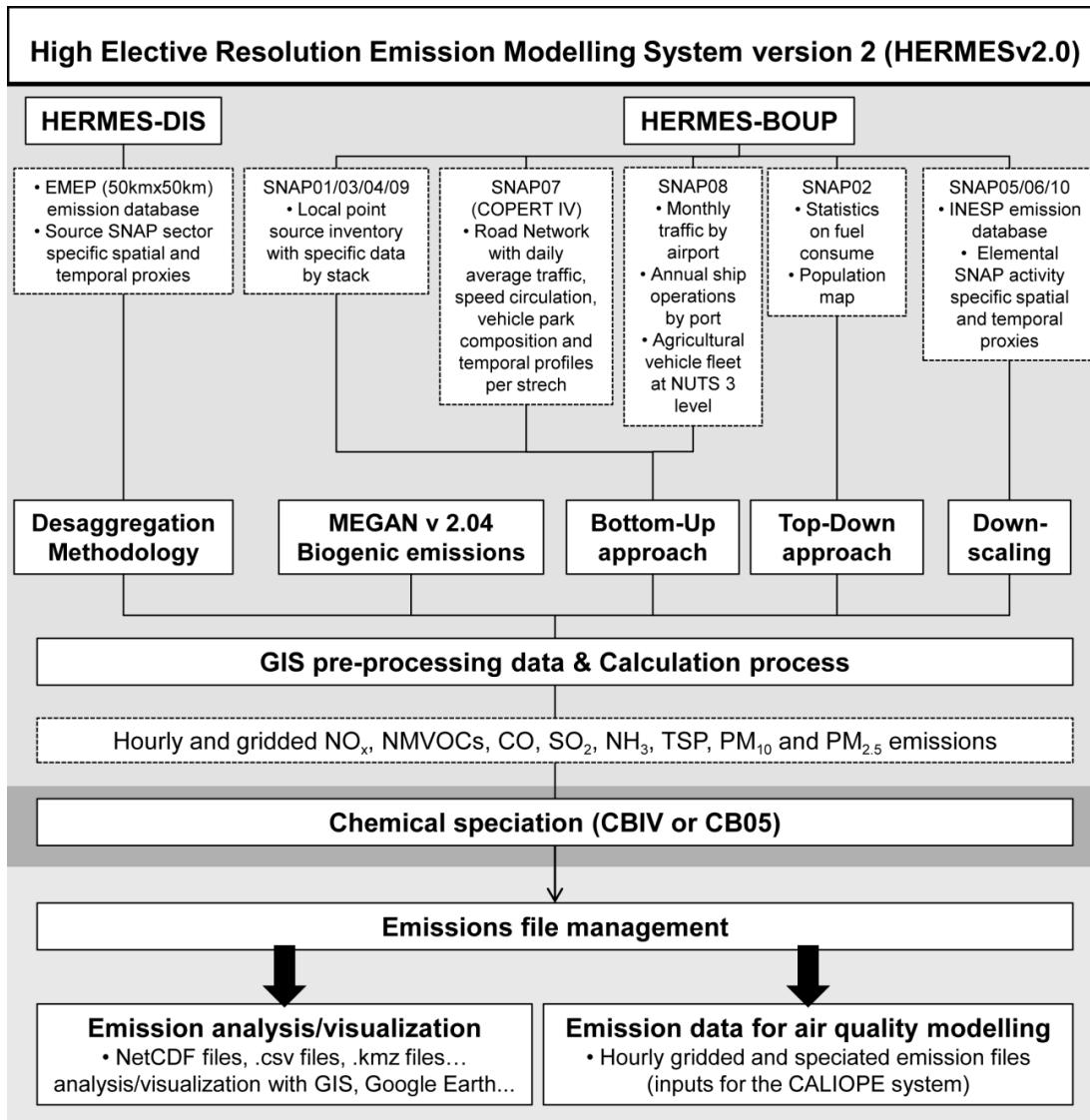
3 online or climatological oxidants (OH, O₃, HO₂)

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

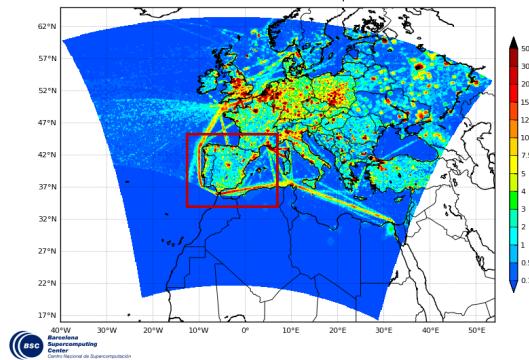
aqueous-phase oxidation by H₂O₂ and O₃



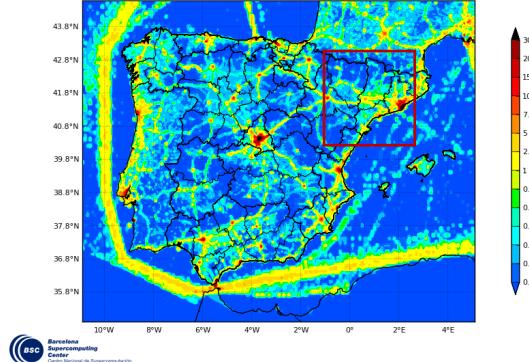
HERMESv2.0: An emission model for Europe and Spain



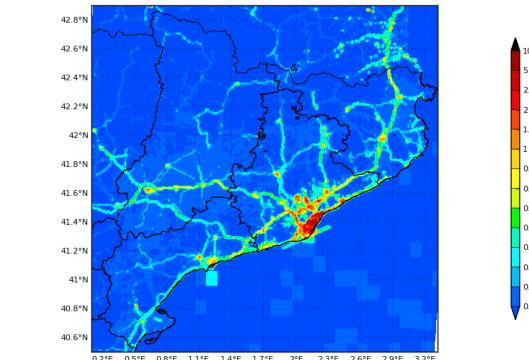
BSC-ES/EMEP disag. by HERMES v.2 Emissions NO₂ (kg/h)
Emissions for 20UTC 25 Feb 2015 - Europe Res: 12x12km



BSC-ES/HERMESv2 Emissions NO₂ (kg/h)
Emissions for 40UTC 26 Feb 2015 - Iberian Peninsula Res: 4x4km



BSC-ES/HERMESv2 Emissions NO₂ (kg/h)
Emissions for 08UTC 25 Feb 2016 - Catalonia Domain Res: 1x1km



- 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

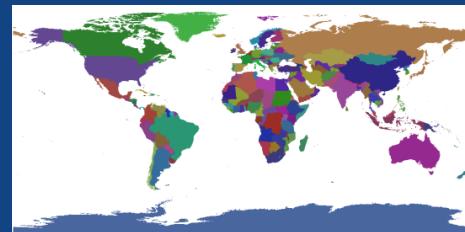
- Multiple **global and regional emission inventories**
- **Online emissions:**
 - Biogenic (MEGAN), lightning, ocean
- Spanish bottom- up emission inventory (street level emissions)



(...)

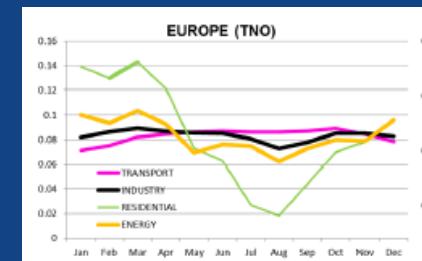
Conservative regridding

- **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



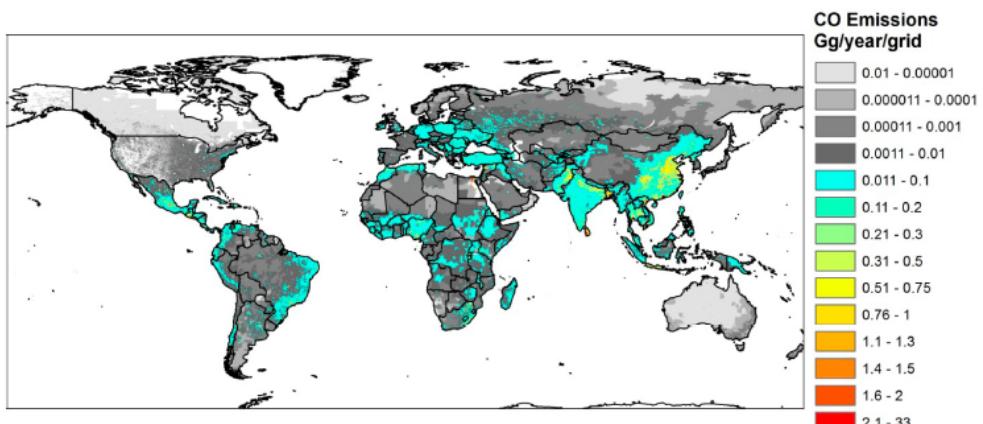
El	Sector	Year	Pollutants	Vertical	Temporal
GFASv1.2 Kaiser et al. (2012)	Biomass burning	2015	oc, bc(*), so2, pm25,c2h6s	Plume top = Sofiev et al. (2012) Distribution=50 % top 50% uniform below	Daily
HTAPv2.2 Janssens- Maenhout et al. (2015)	energy	2010	oc, bc, so2, pm25, pm10	218-724 m (Bieser et al., 2011)	Monthly
	industry			72-292 m (Bieser et al., 2011)	
	residential			First layer	
	transport			First layer	
	air_lto			0 – 1 km	Yearly (monthly flat profile)
	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)

Residential waste burning

- **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

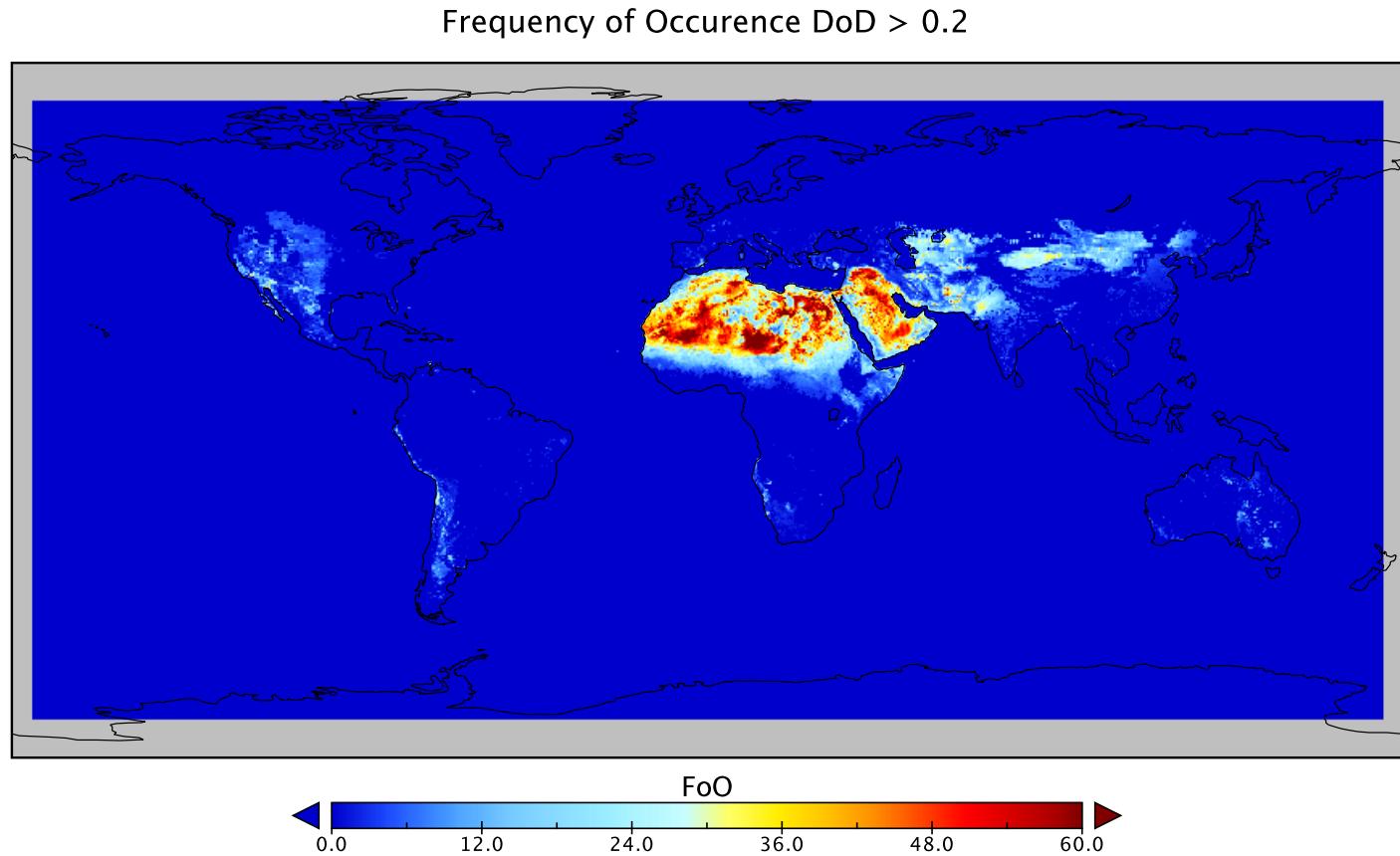


Wiedinmyer et al. (2014)

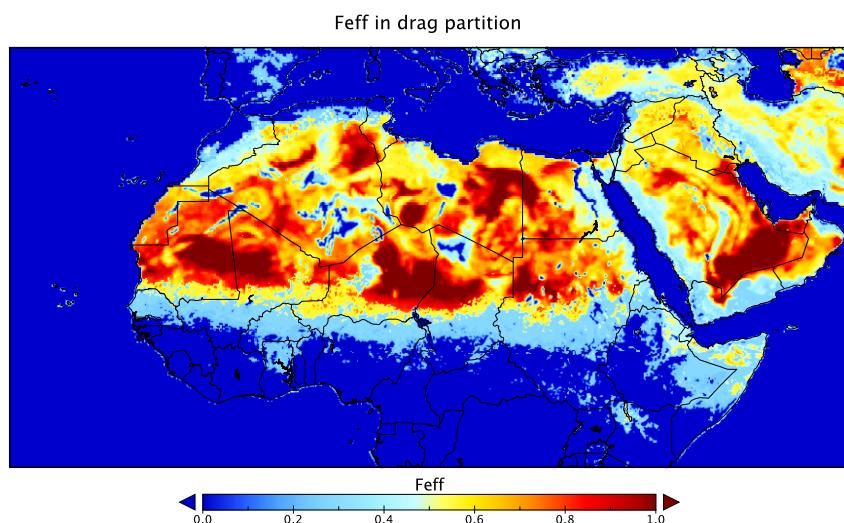
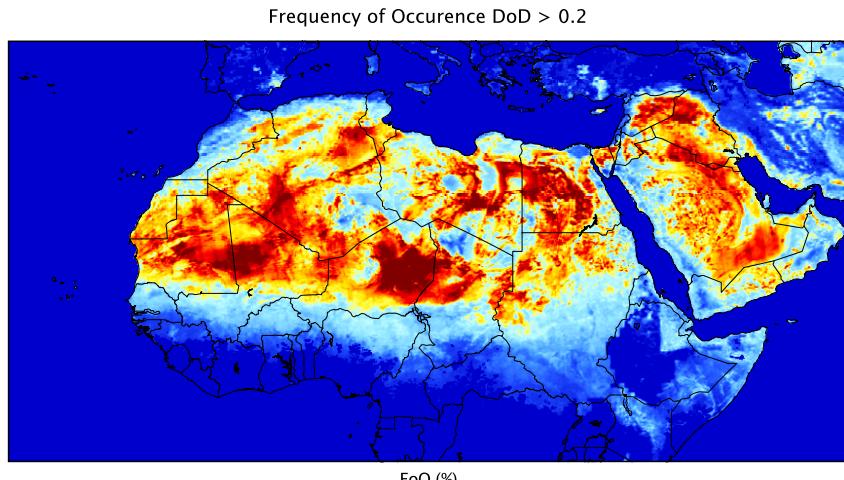
**For this sector, PM_{2.5}-BC-OC accounts
for 42.7% of total PM_{2.5}.
All PM_{2.5}-BC-OC is considered PMFINE**

Natural aerosol emissions

- 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



Natural aerosol emissions



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

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

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

AOD Evaluation 2015

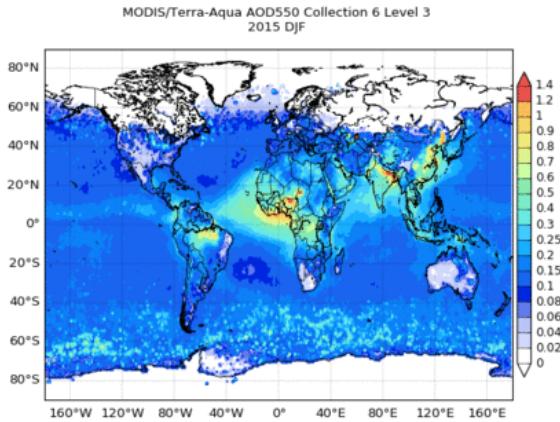


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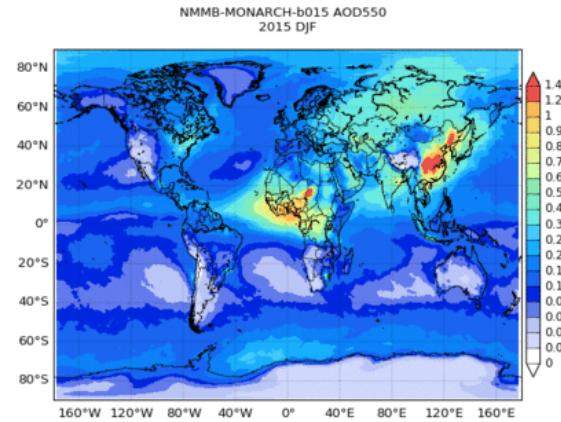
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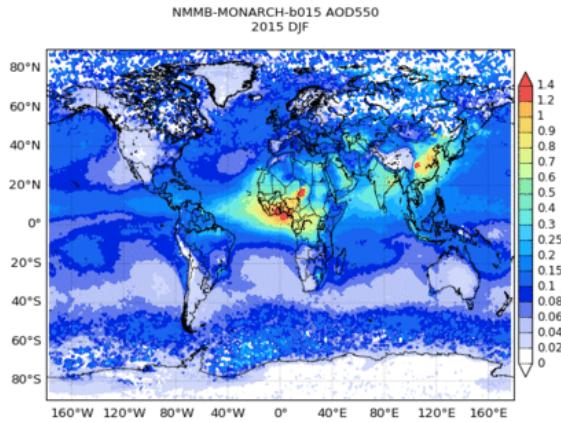
MODIS C6 Level 3



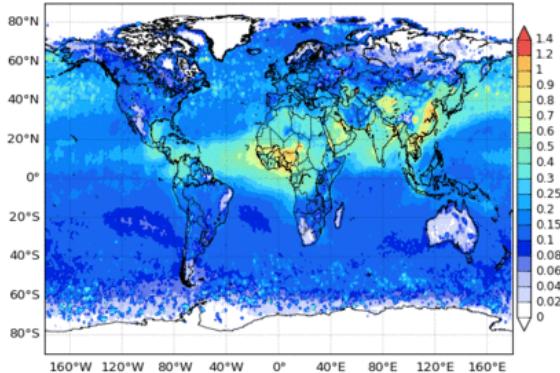
MONARCH All Sky



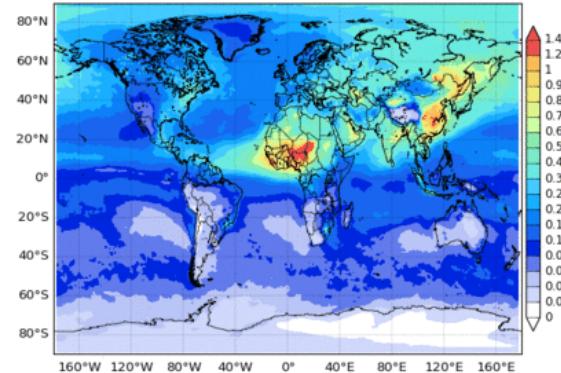
MONARCH Clear Sky



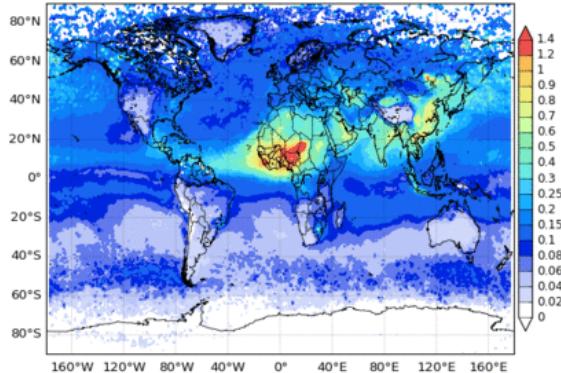
MODIS/Terra-Aqua AOD550 Collection 6 Level 3
2015 MAM



NMMB-MONARCH-b015 AOD550
2015 MAM



NMMB-MONARCH-b015 AOD550
2015 MAM



AOD Evaluation 2015



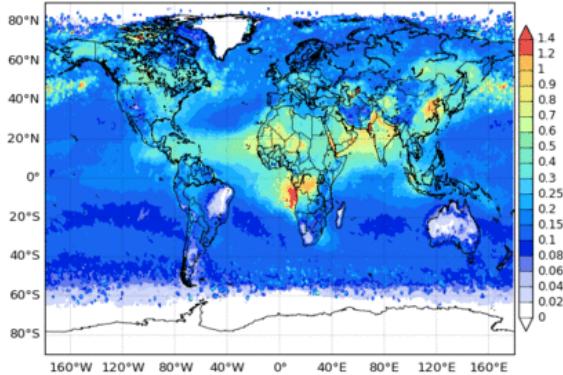
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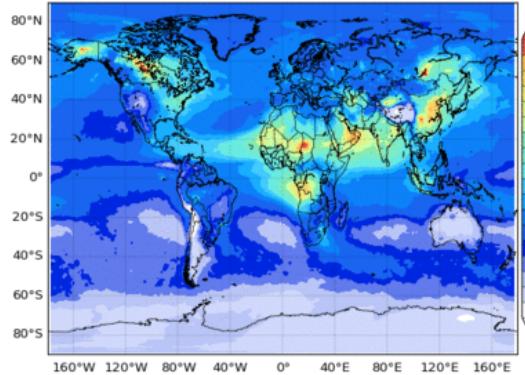
MODIS C6 Level 3

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



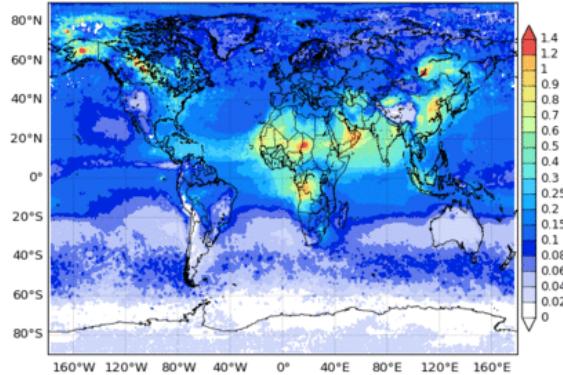
MONARCH All Sky

NMMB-MONARCH-b015 AOD550
2015 JJA

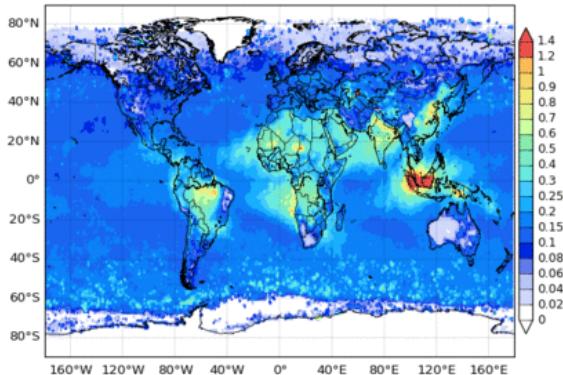


MONARCH Clear Sky

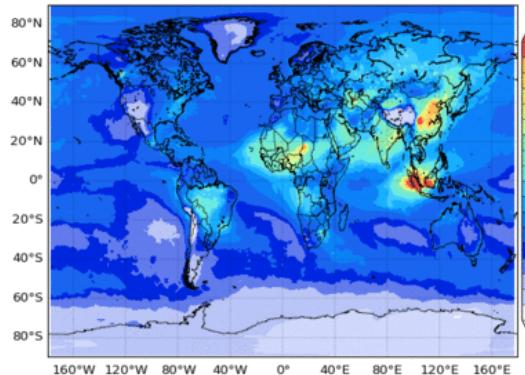
NMMB-MONARCH-b015 AOD550
2015 JJA



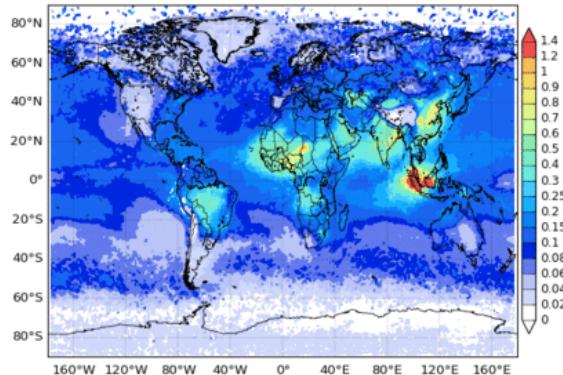
MODIS/Terra-Aqua AOD550 Collection 6 Level 3
2015 SON



NMMB-MONARCH-b015 AOD550
2015 SON



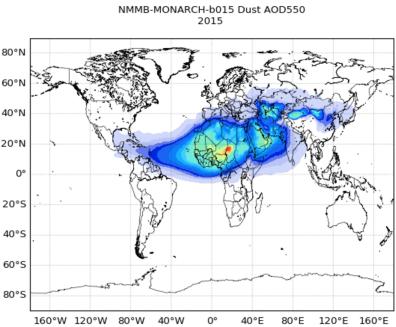
NMMB-MONARCH-b015 AOD550
2015 SON



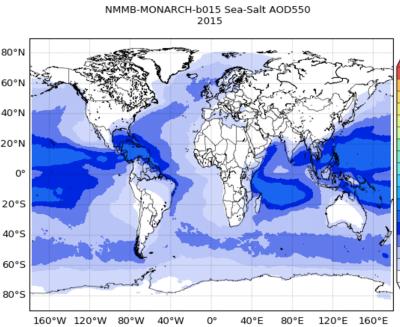
AOD components



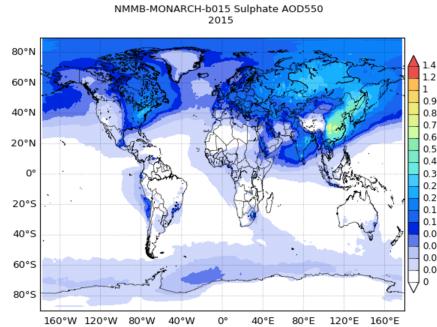
Dust



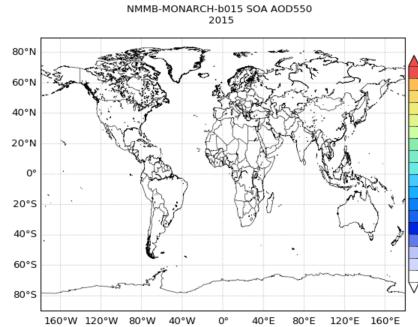
SS



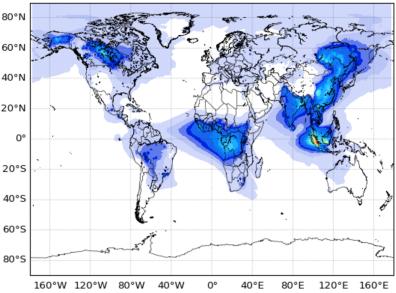
SU



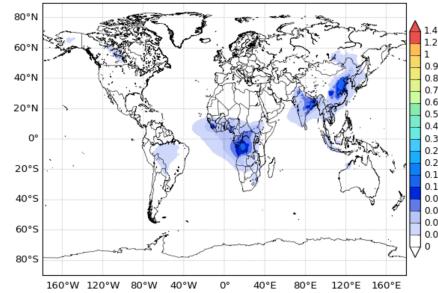
SOA



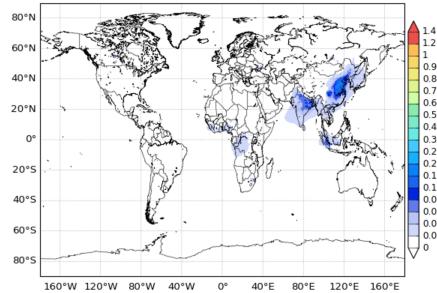
NMMB-MONARCH-b015 Organic Matter AOD550
2015



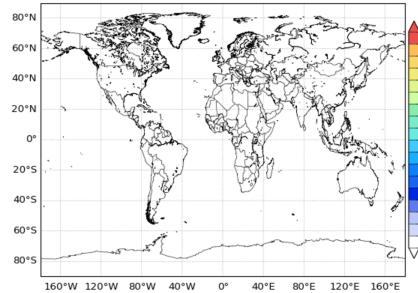
NMMB-MONARCH-b015 Black Carbon AOD550
2015



NMMB-MONARCH-b015 Unspecified fine AOD550
2015



NMMB-MONARCH-b015 Unspecified coarse AOD550
2015



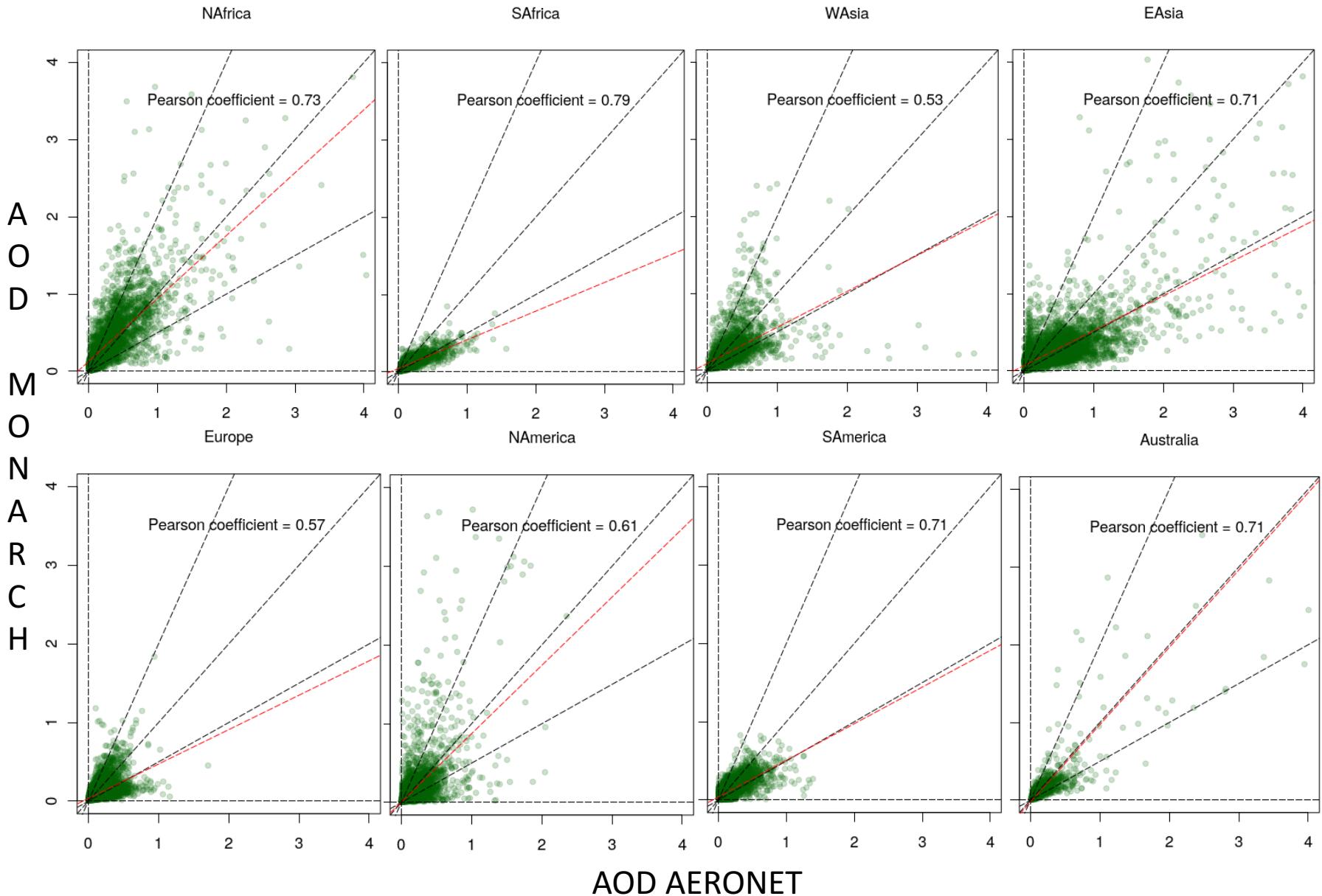
OM

BC

Fine (unspec.)

Coarse (unspec.)

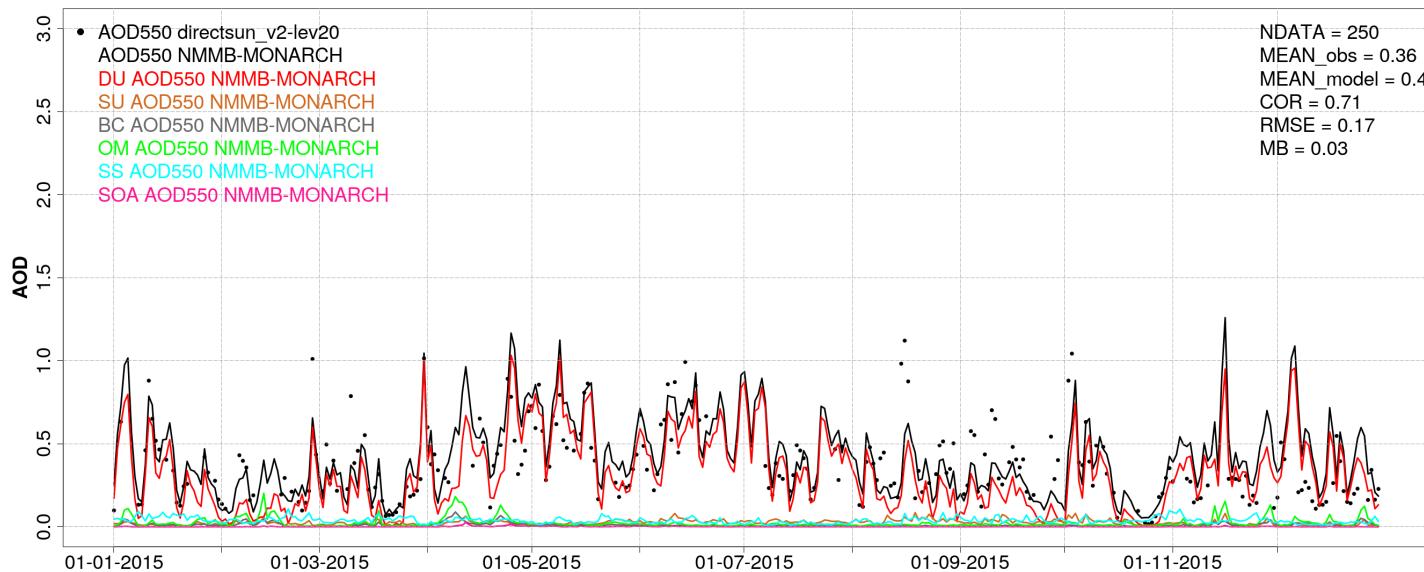
AOD Evaluation 2015



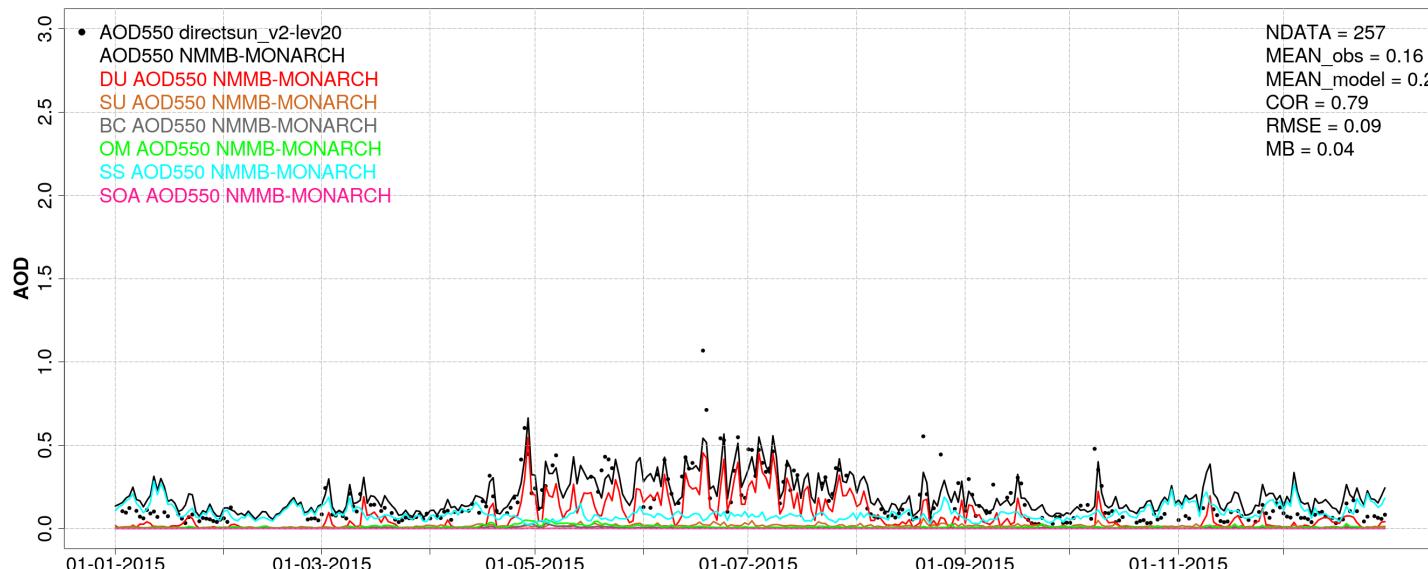
Dust Atlantic Transport

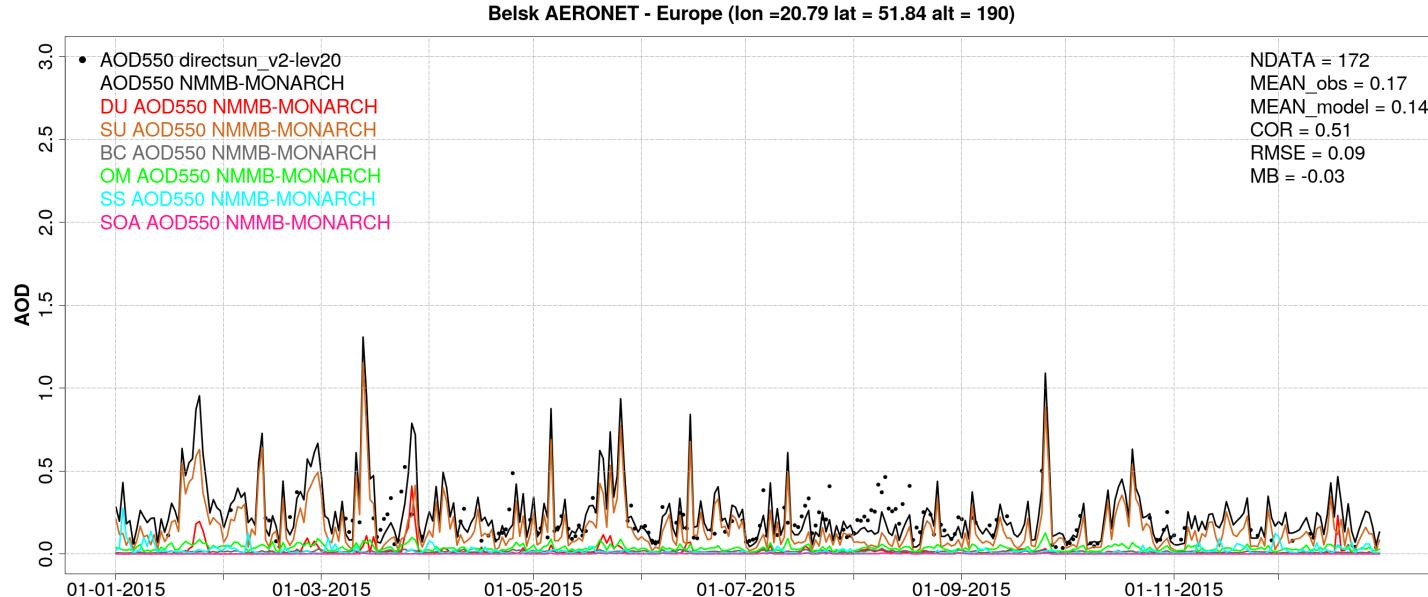
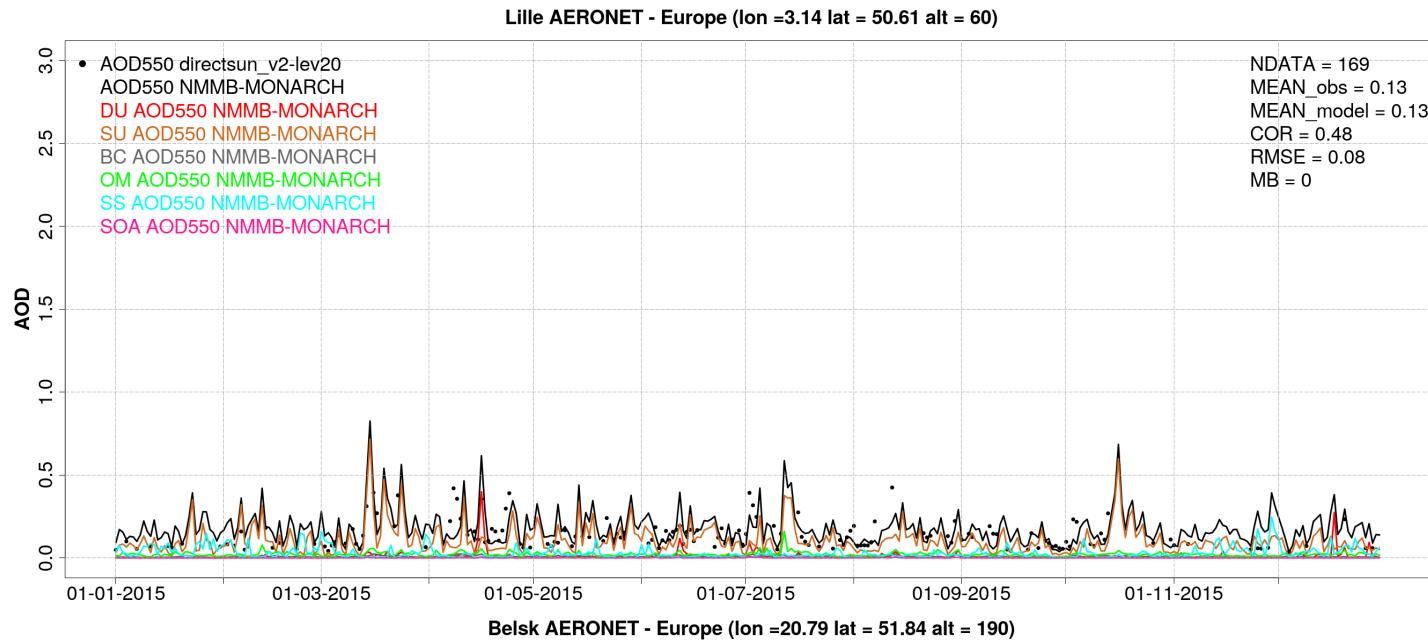


Capo_Verde AERONET - NAfrica (lon =-22.94 lat = 16.73 alt = 60)



Guadeloupe AERONET - SAmerica (lon =-61.5 lat = 16.33 alt = 0)





Biomass Burning

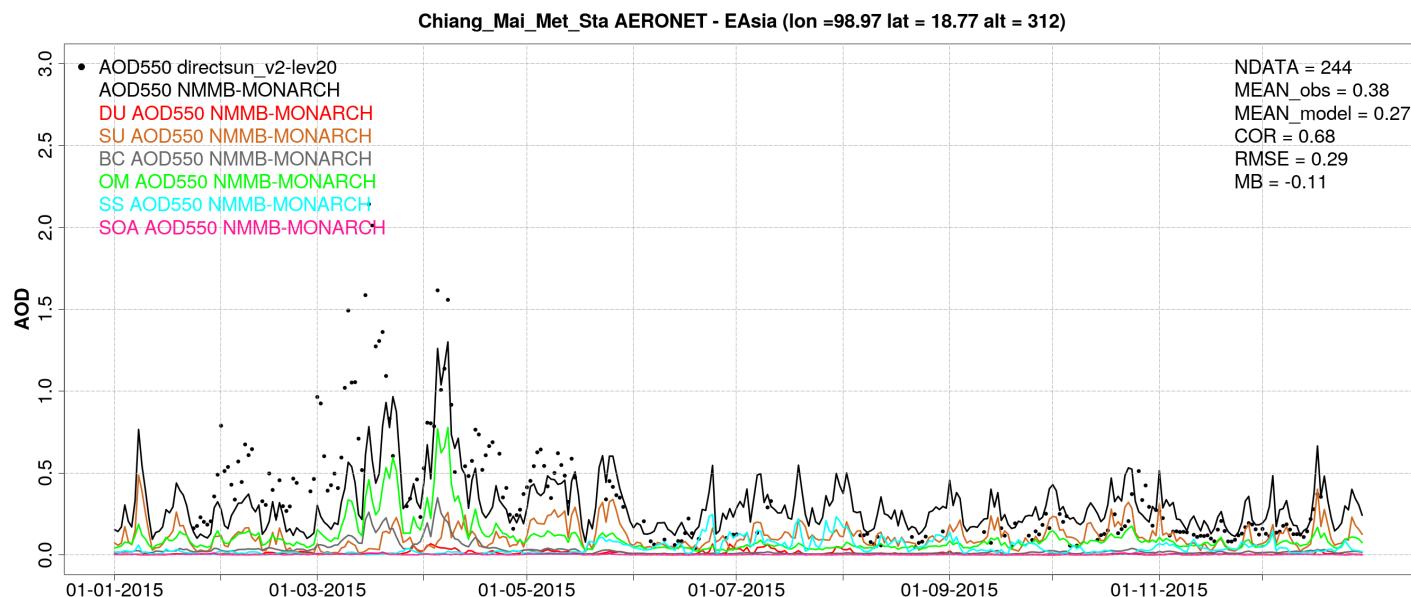
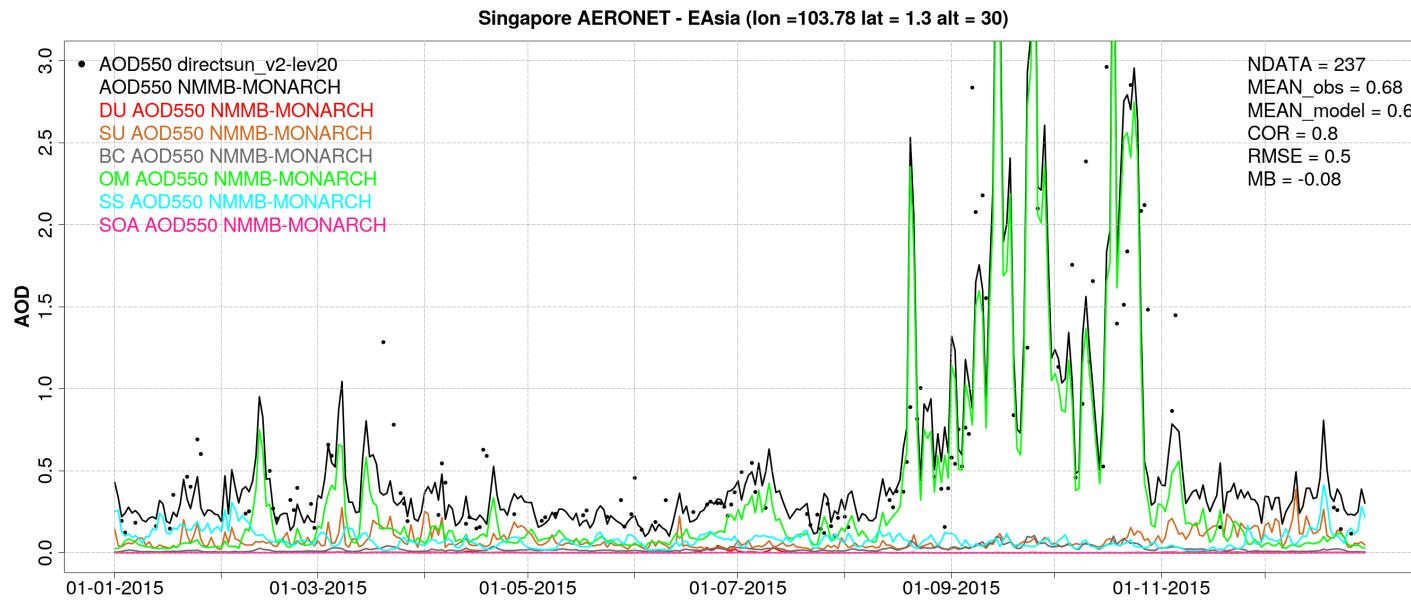


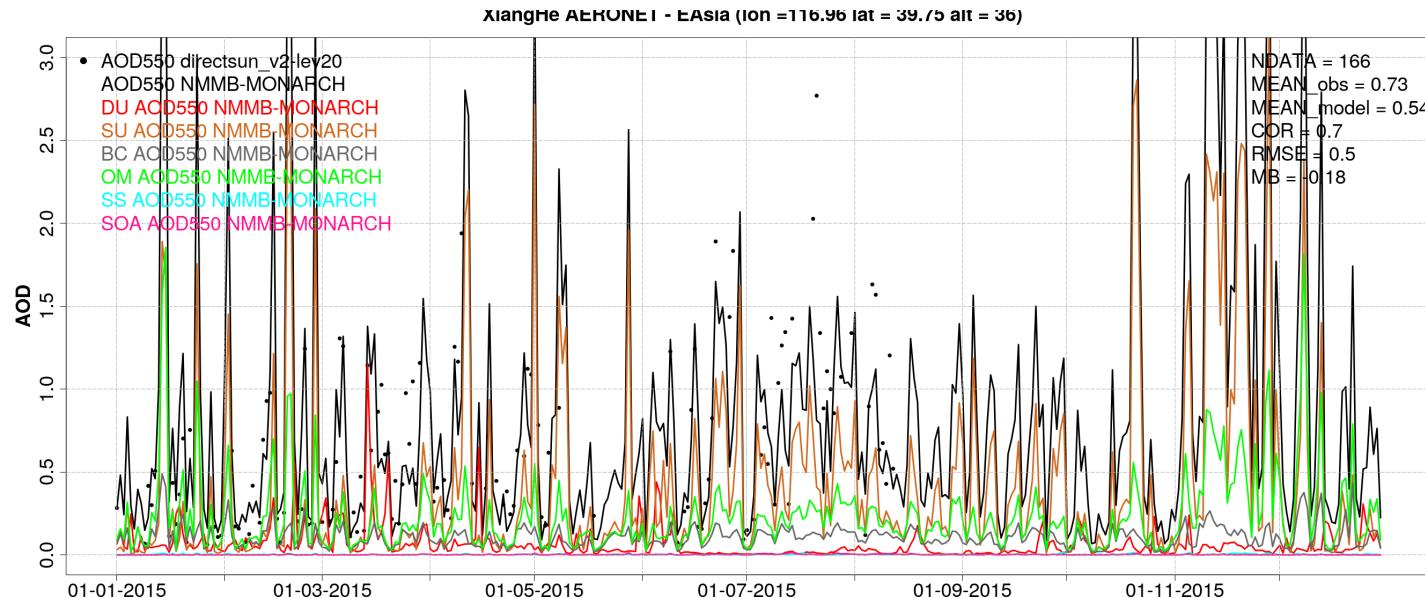
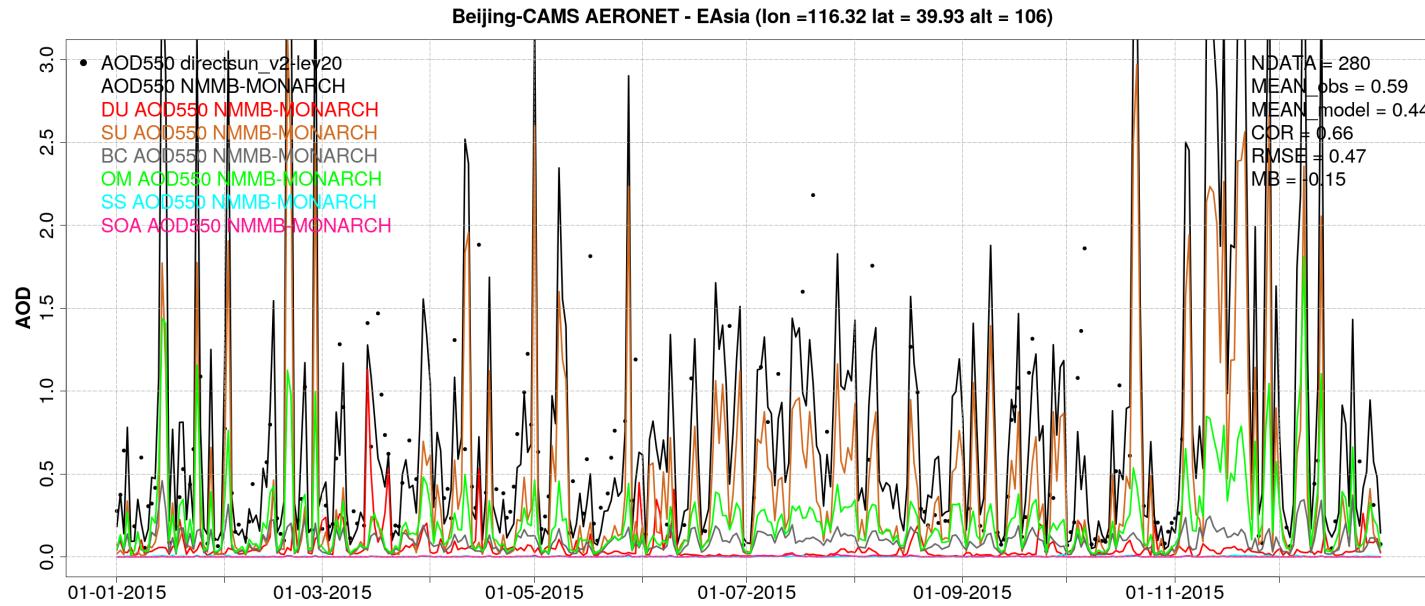
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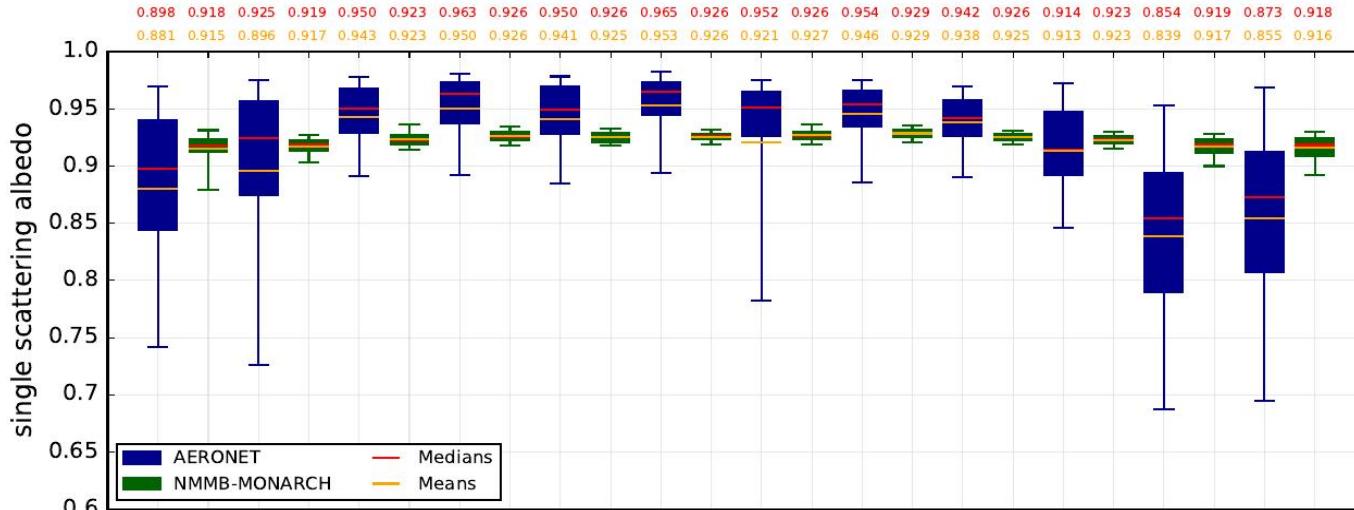


Intensive Optical Properties in MONARCH



- Preliminary results of evaluation against AERONET of aerosol single scattering albedo simulated by the MONARCH:

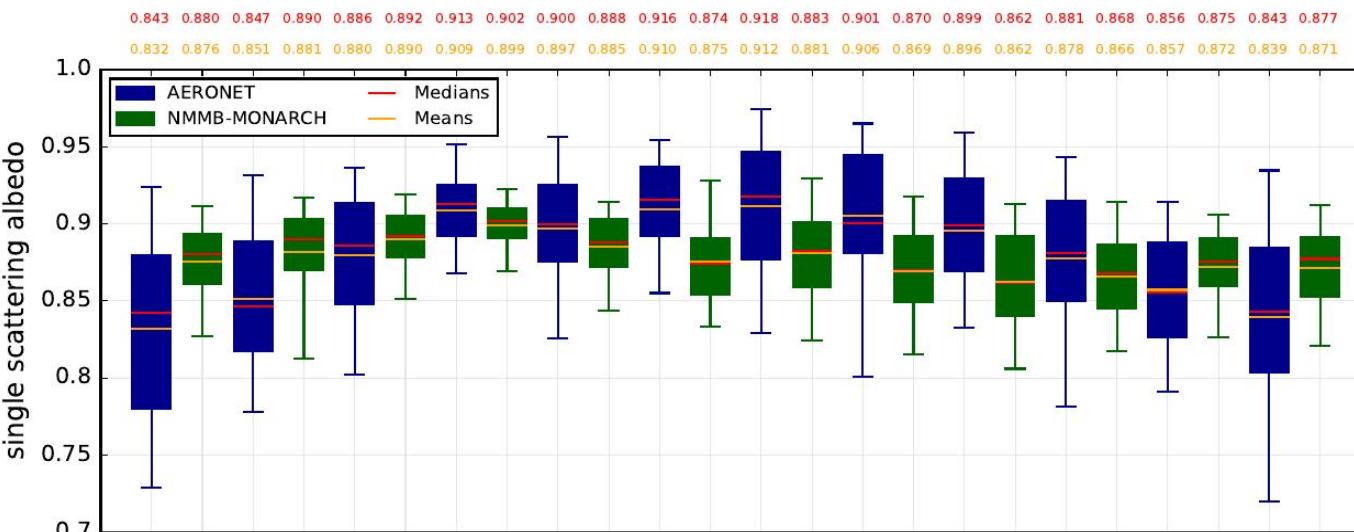
Agoufou (lev 1.5 - screened); lon: -1.479, lat: 15.345, h (m): 305.000



i) AERONET level 1.5 data with all screening 2.0 filters applied except AOD > 0,4

ii) Monthly data collected over 5 years (2002-2006): # measures > 30 for each month

Beijing (lev 1.5 - screened); lon: 116.381, lat: 39.977, h (m): 92.000

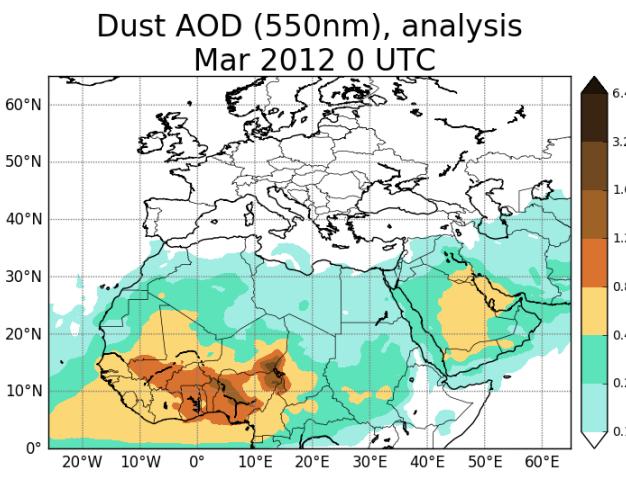
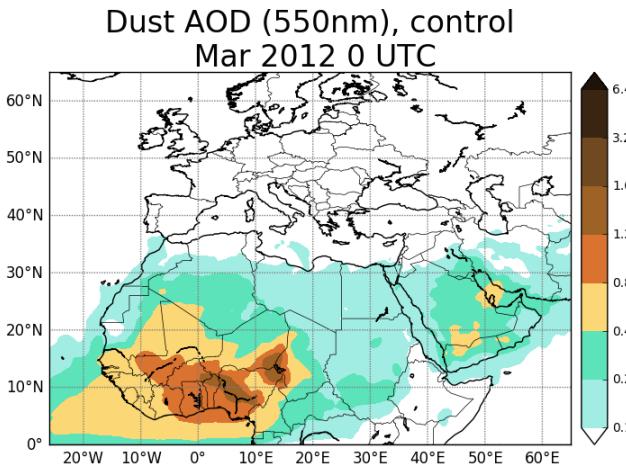


- Testing new observational datasets (**MODIS coarse DB, IASI dust AOD**)
- Vertical observational constraint (assimilation of extinction profiles)
- Multi-scale capability (coping with a limited area domain and rotated coordinate system, e.g. used by the BDFC)
- Adapting the DA scheme to model developments (**MONARCH v2.0**)

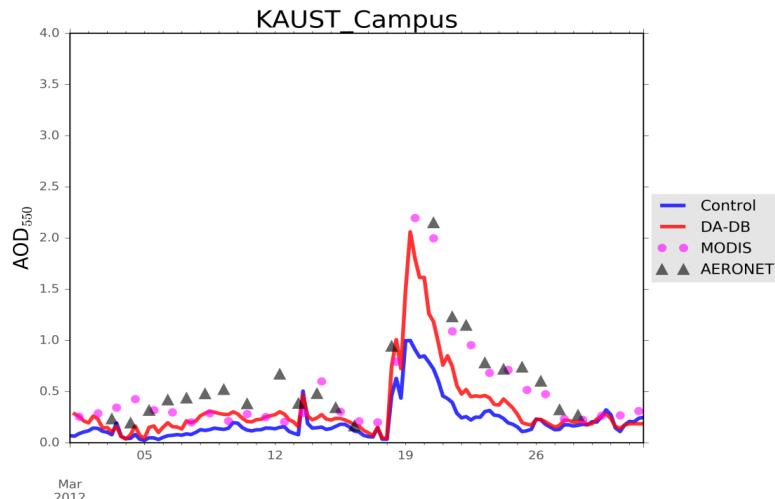
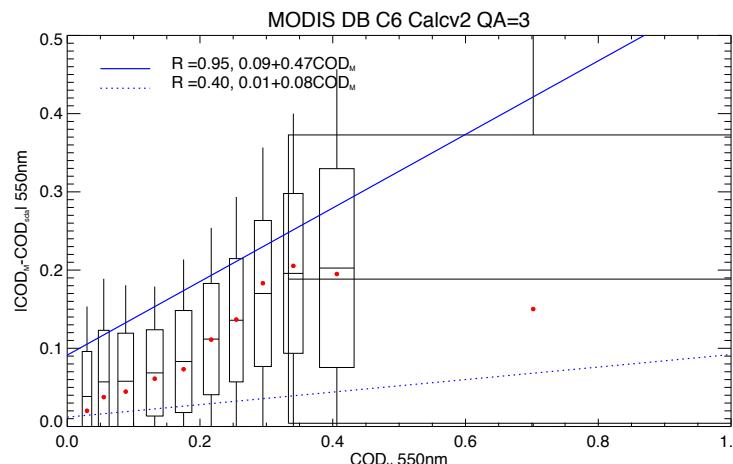
MODIS Deep Blue coarse DoD

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



Error estimates: collocated comparison of DOD over N Africa (5 to 35N, -20 to 60E) with AERONET data between 2003 and 2015



Assimilation of MODIS coarse Deep Blue

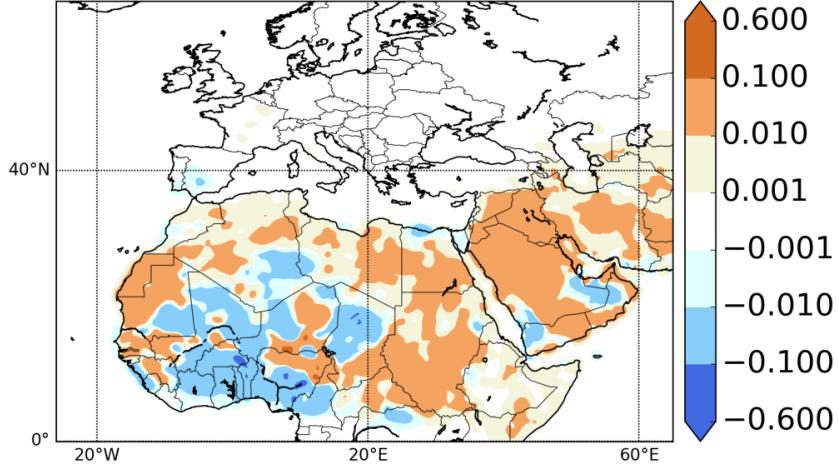


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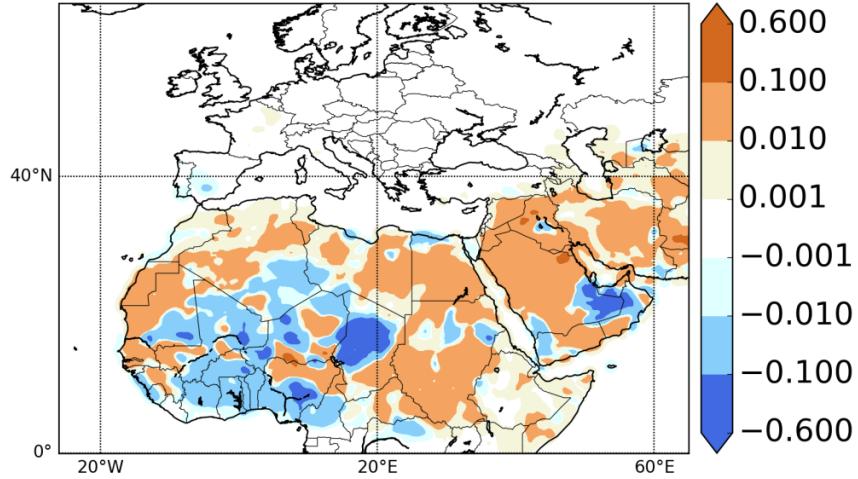


Feedback from assimilation increments

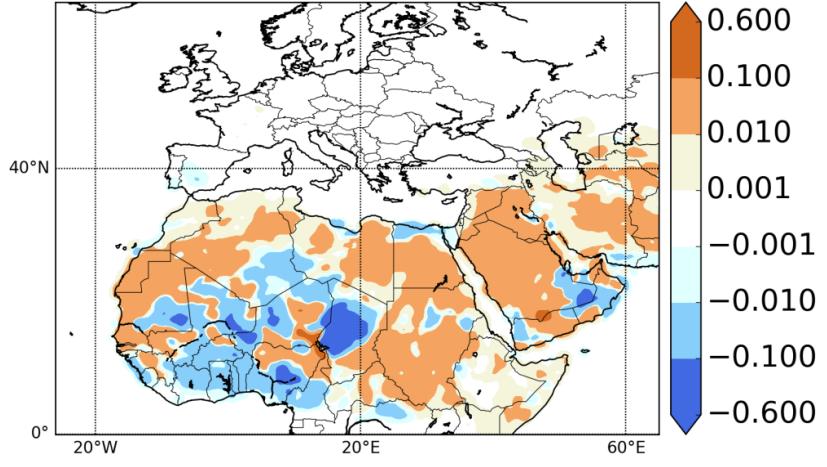
Dust AOD (550nm) analysis - first guess
Mar 2015 6 UTC



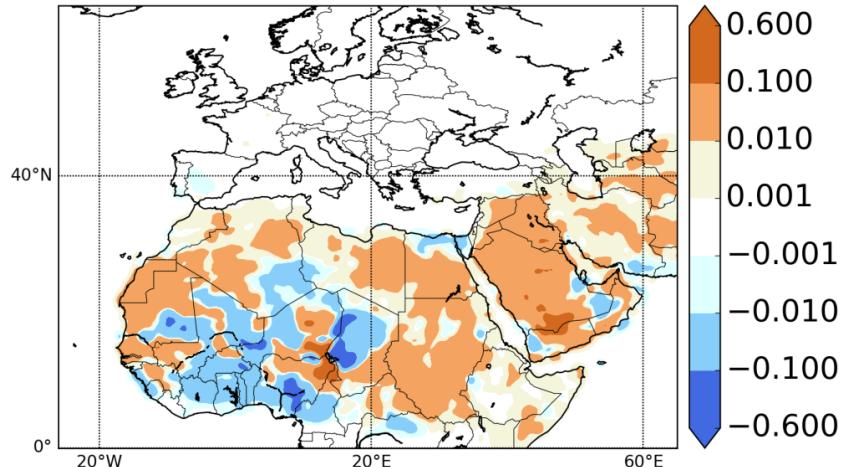
Dust AOD (550nm) analysis - first guess
Mar 2015 12 UTC



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

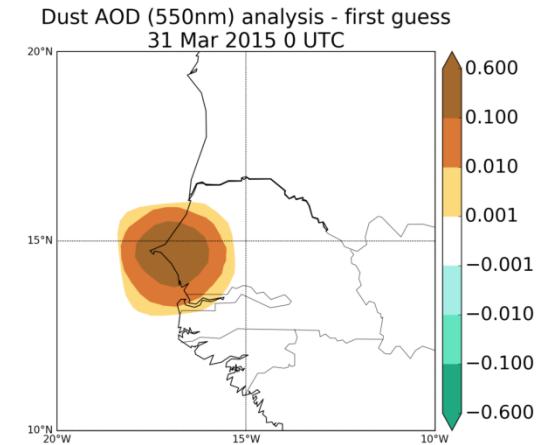
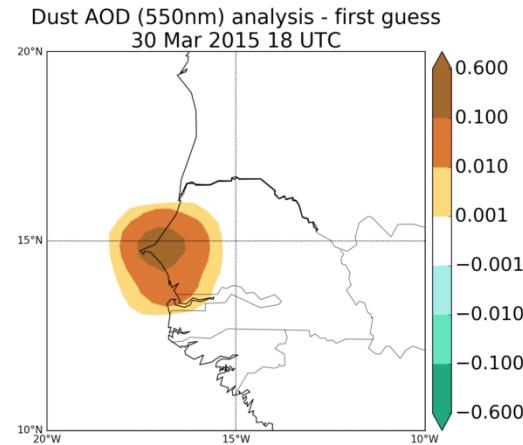
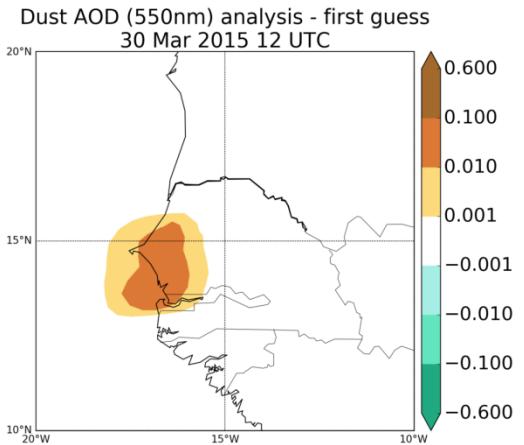
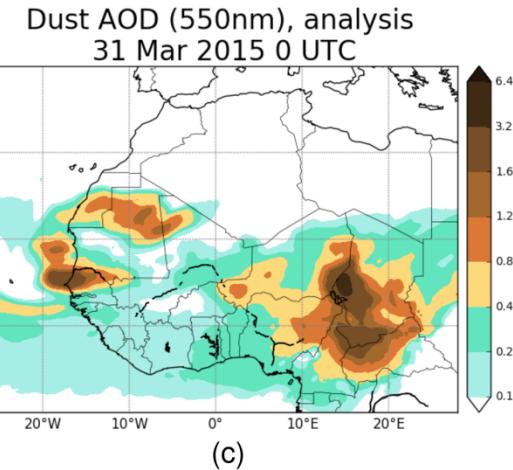
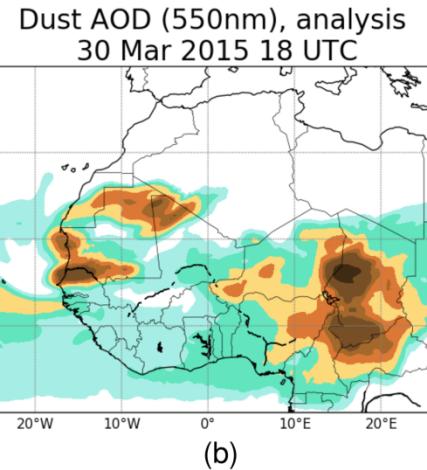
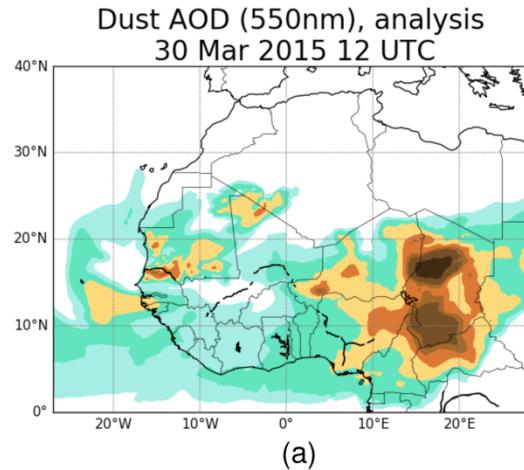


Dust AOD (550nm) analysis - first guess
Mar 2015 0 UTC



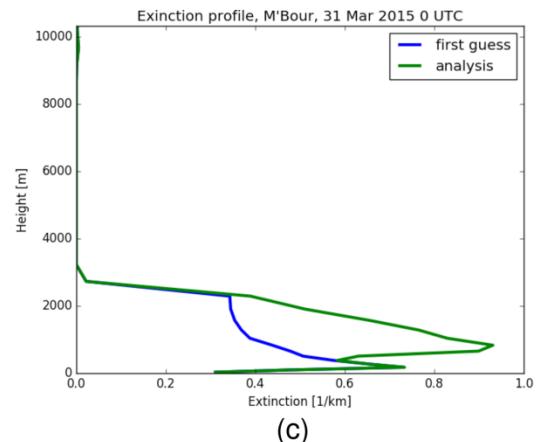
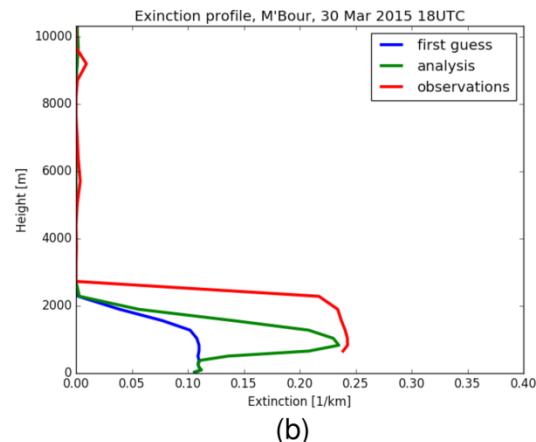
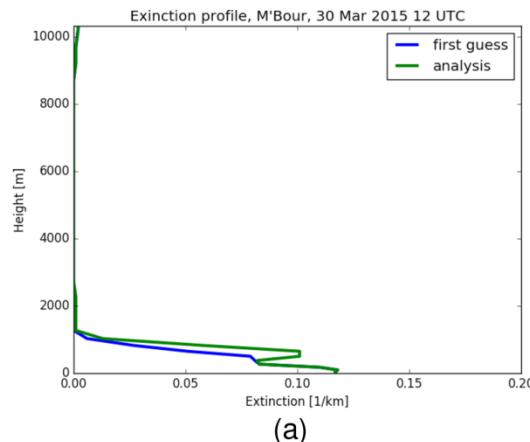
Evaluating the potential of ACTRIS-2 data for assimilation through pilot dust case studies

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

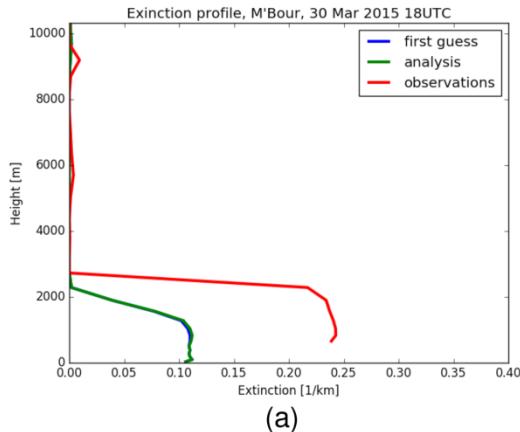


Evaluating the potential of ACTRIS-2 data for assimilation through pilot dust case studies

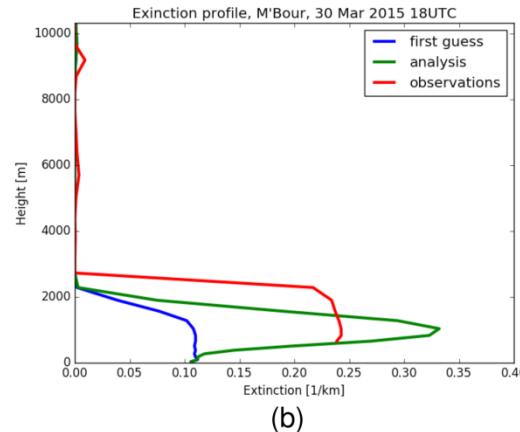
Observational impact through the whole assimilation window



Higher observation uncertainty



Increasing the vertical localization factor

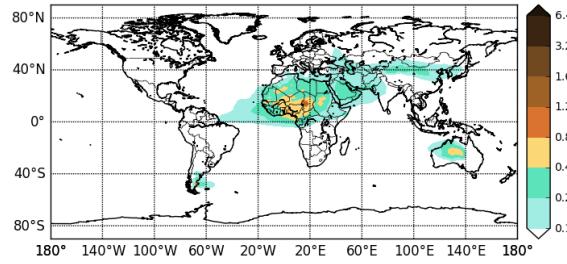


Case Study ESA Climate Change Initiative

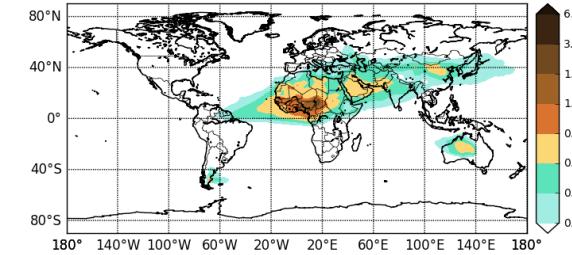


IASI dust reanalyses (MetOp-A IASI in the thermal IR)

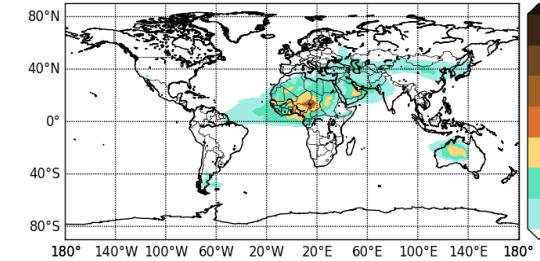
Dust AOD (550nm), DA Simulation (ULB)
March 2015



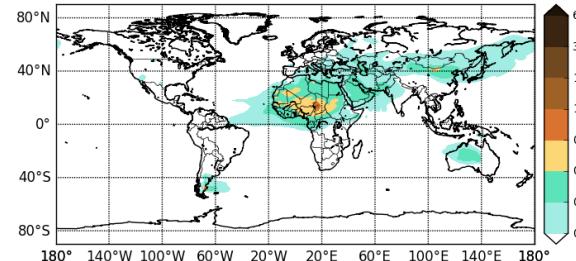
Dust AOD (550nm), DA Simulation (MAPIR)
March 2015



Dust AOD (550nm), DA Simulation (IMARS)
March 2015



Dust AOD (550nm), DA Simulation (LMD)
March 2015



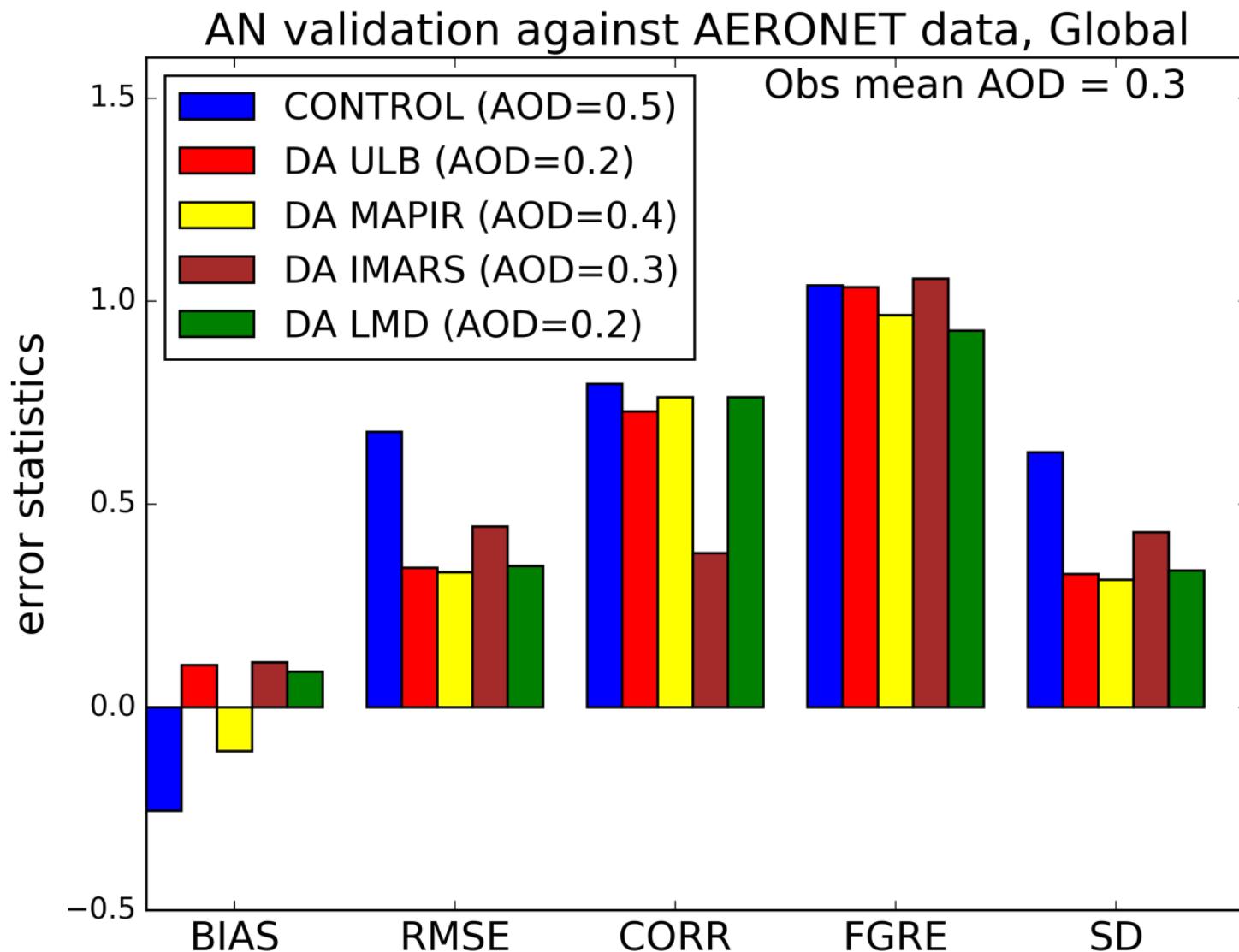
Level 3 mineral dust AOD datasets

- retrieved from MetOp-A IASI in the **thermal IR**
- uncertainty estimation
- converted to 550nm
- sub-daily set mineral dust retrievals (6h)
- spatially aggregated (1x1)
- screened for AOD (>0.15)

4 different retrieval algorithms

- ULB v7, Universite Libre de Bruxelles
- MAPIR v3.5, BIRA-IASB
- LMD v2.1
- IMARS v5.2, DLR

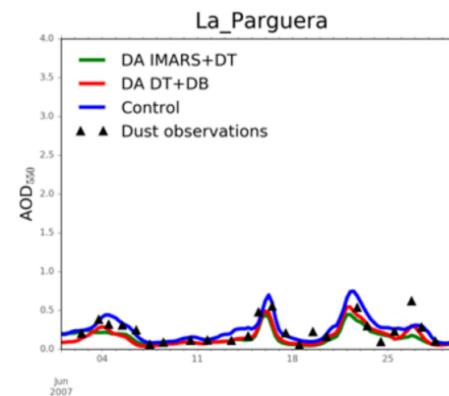
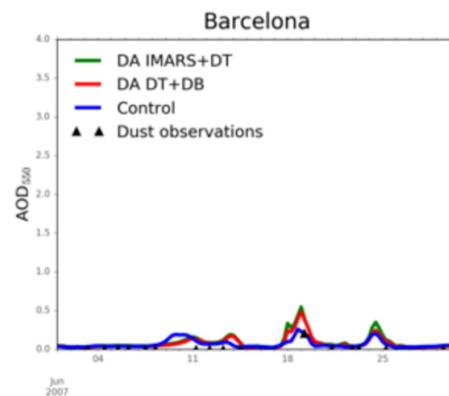
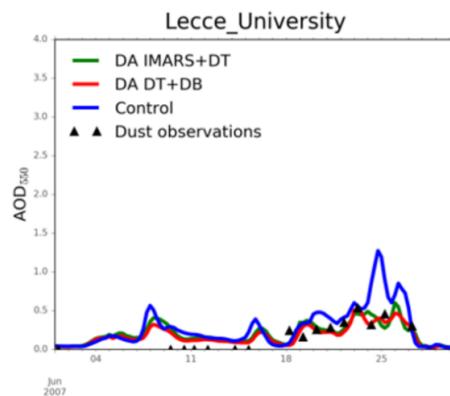
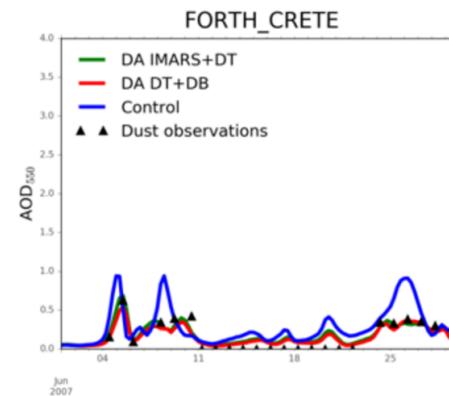
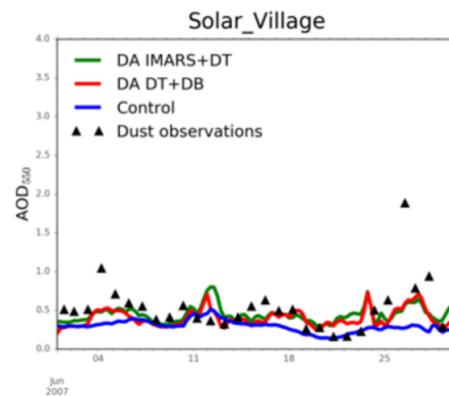
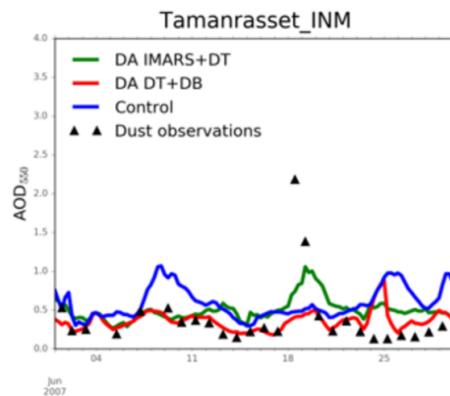
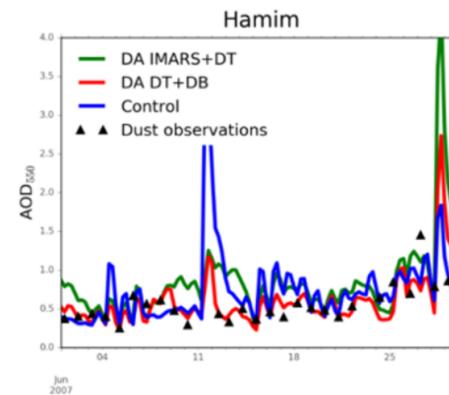
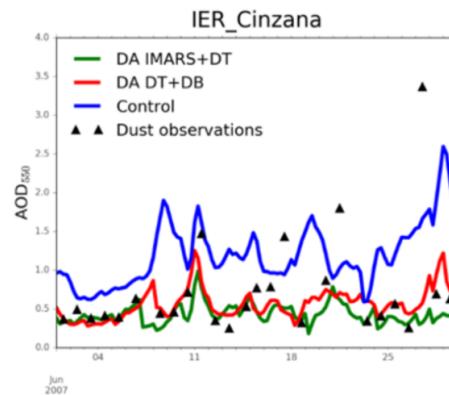
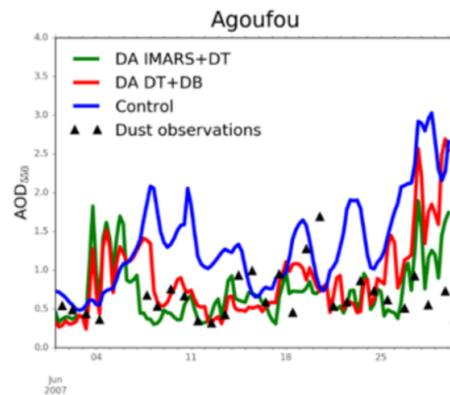
Case Study ESA Climate Change Initiative



Case Study ESA Climate Change Initiative



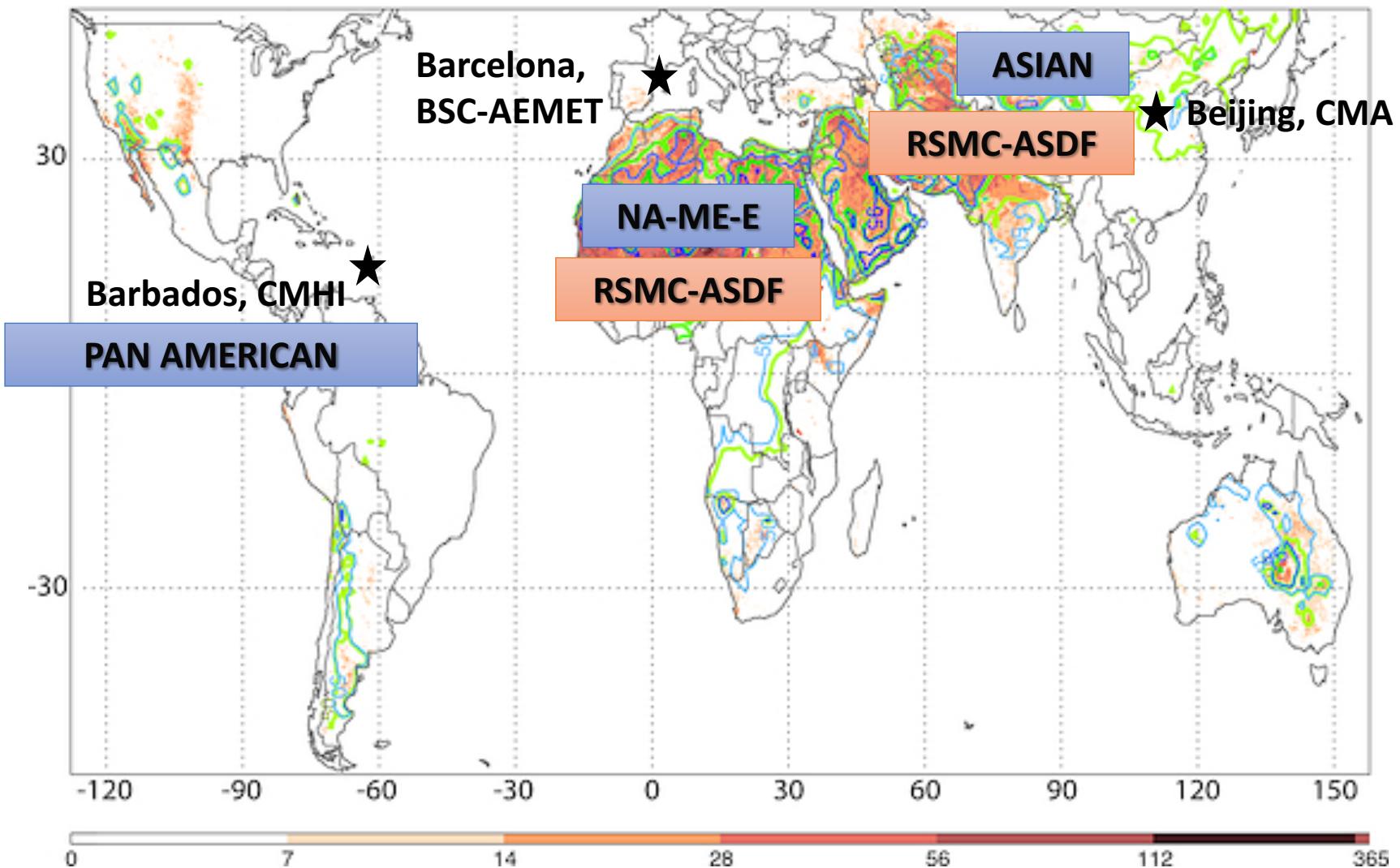
IMARS_QC
+
DT



WMO Dust Regional Centers



Barcelona
Supercomputing
Center
Centro Nacional de Supercomputación



WMO Dust Centers in BCN

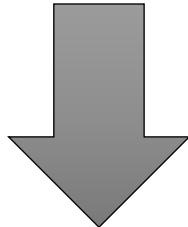


Barcelona
Supercomputing
Center
Centro Nacional de Supercomputación



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

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

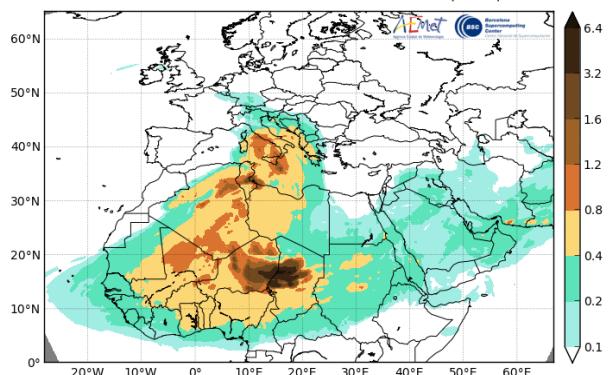


Barcelona Dust Forecast Center - Operations
First specialized WMO Center for mineral dust prediction. Started in 2014

[@Dust_Barcelona](http://dust.aemet.es)



Barcelona Dust Forecast Center - <http://dust.aemet.es/>
NMMB/BSC-Dust Res:0.1°x0.1° Dust AOD
Run: 12h 11 MAY 2016 Valid: 12h 11 MAY 2016 (H+00)



SDS-WAS NAMEE: Dust observations



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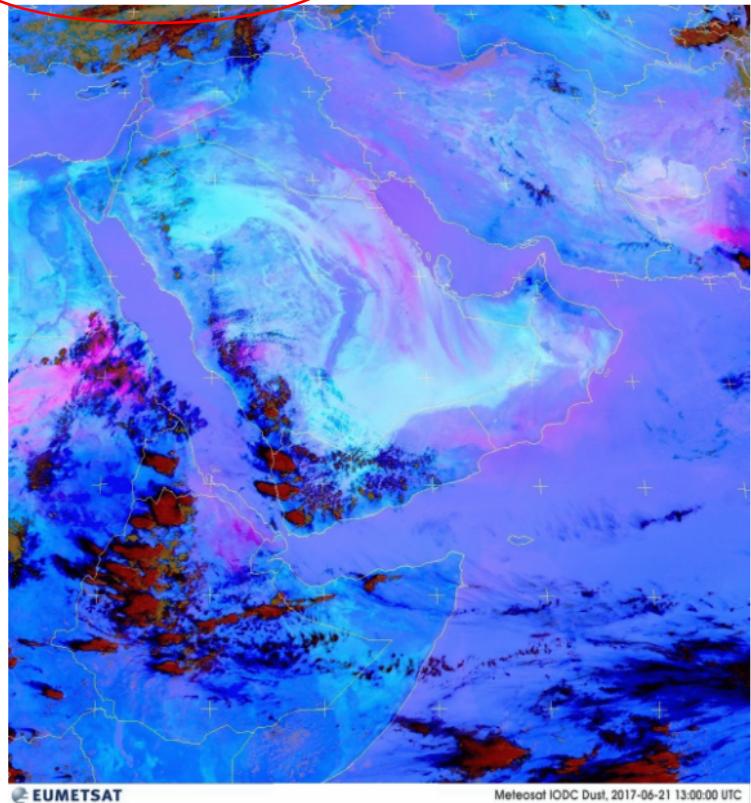


MSG – EUMETSAT Middle East

by Francesco Bevilacqua — last modified Mar 17, 2017 11:32 AM

Date: 2017-06-21

Archive



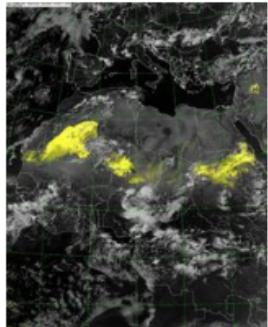
[Download full image](#)



DEBRA-Dust

by Enric Terradellas — last modified Mar 22, 2017 03:30 PM

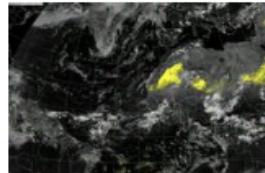
MSG - Africa



[Latest image](#)
[5-hour loop](#)
[4-week archive](#)

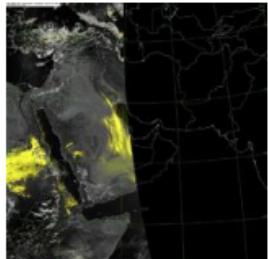


MSG - Atlantic



[Latest image](#)
[5-hour loop](#)
[4-week archive](#)

Suomi NPP VIIRS - West Asia



[Latest image](#)
[3-day loop](#)
[4-week archive](#)



<http://sds-was.aemet.es/> 31

SDS-WAS NAMEE: Towards NRT Evaluation profiles



OBSERVATIONS

***Extinction profiles at 12UTC
available in a window of 24 hours***



3 ceilometers

1 lidar



SDS-WAS MODELS

- **BSC-DREAM8b**
- **NMMB/BSC-Dust**
- **CAMS**
- **DREAM8-NMME**
-

```
2016040512_3H_BSC_DREAM8B_profiles {  
dimensions:  
    time = 73;
```

Data format
*Exchange operational protocol
includes 72 hours forecasts*

```
lon:long_name = "longitude";  

lon:units = "positive degrees East";  

double lat(station);  

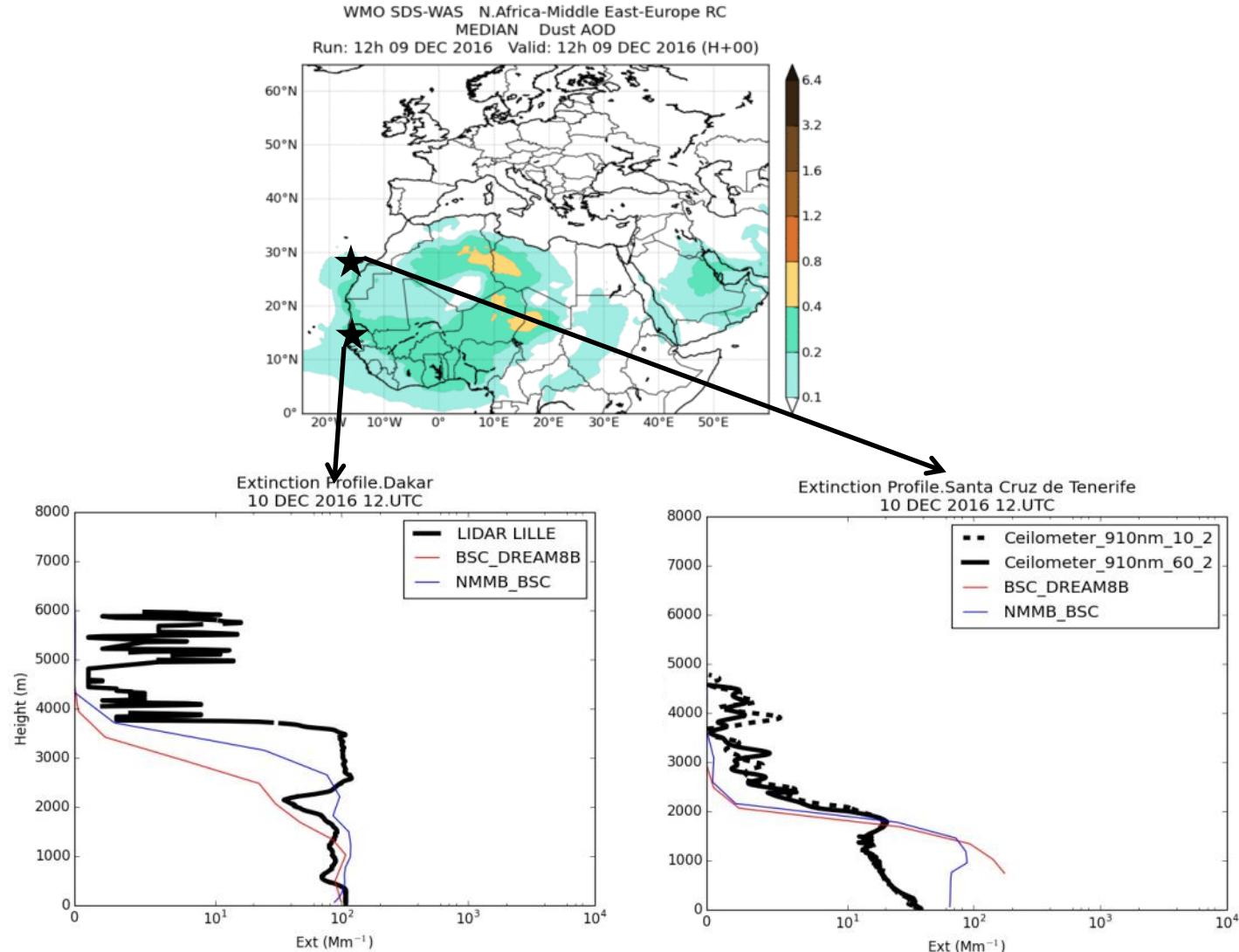
lat:long_name = "latitude";  

lat:units = "positive degrees North";  

char station_name(station, strlen);
```

SDS-WAS NAMEE: NRT Evaluation profiles

Atlantic dust event: 9 - 12 December 2016



SDS-WAS NAMEE: Daily Dust Forecasts

Dust prediction models provide 72 hours (at 3-hourly basis) of dust forecast (AOD at 550nm and surface concentration) covering NAMEE



MODEL	RUN TIME	DOMAIN	DATA ASSIMILATION
BSC-DREAM8b	12	Regional	No
CAMS ECMWF	00	Global	MODIS AOD
DREAM8-NMME	00	Regional	CAMS analysis
NMMB/BSC-Dust	00	Regional	No
MetUM	12	Global	MODIS AOD
GEOS-5	00	Global	MODIS reflectances
NGAC	00	Global	No
RegCM4 EMA	00	Global	No
DREAMABOL	12	Regional	No
WRF-CHEM NOA	12	Regional	No
SILAM	12	Regional	No
LOTOS-EUROS	12	Regional	No

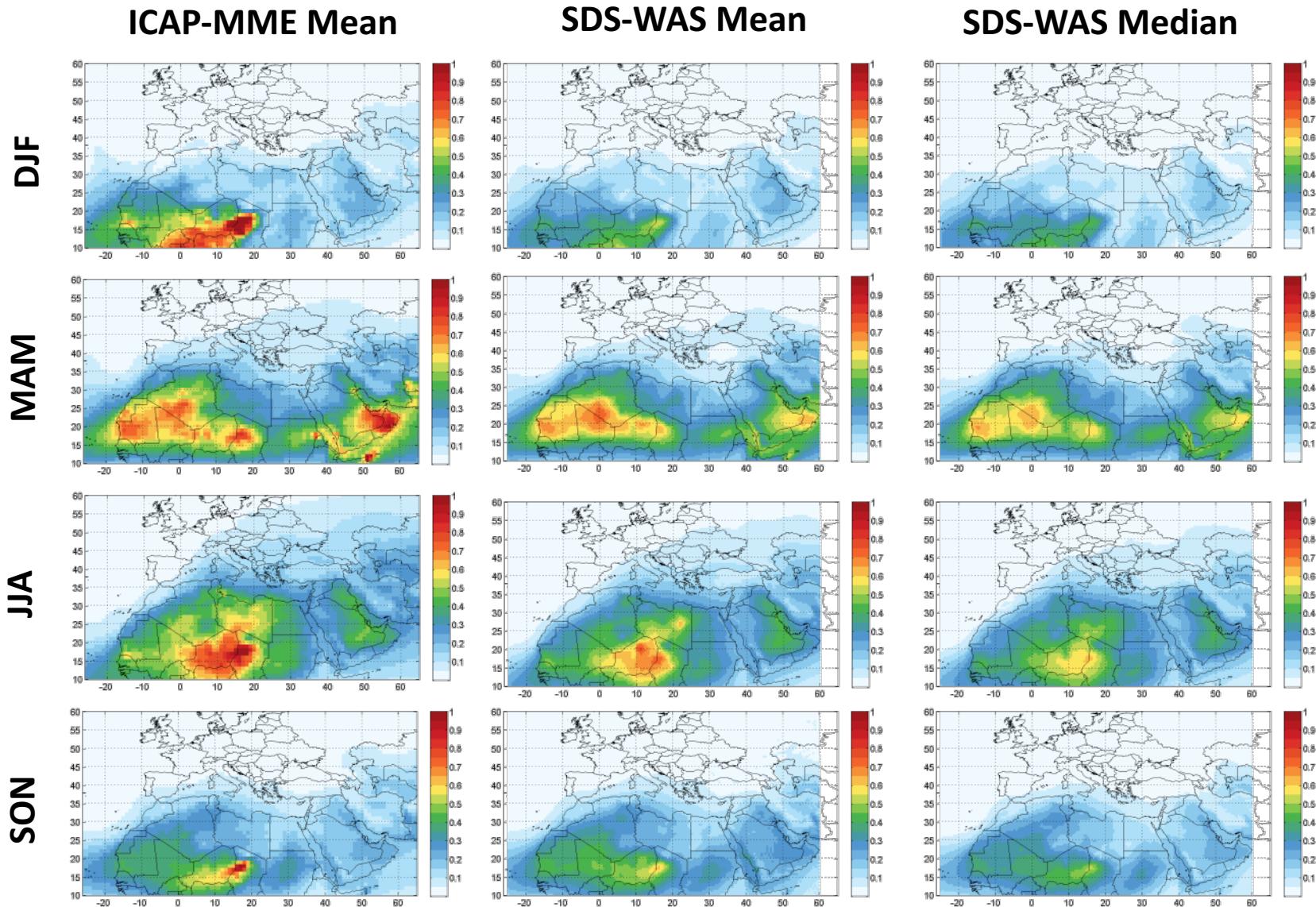
ICAP-MME vs SDS-WAS: Results 2016



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SEVERO
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Centro Nacional de Supercomputación



ICAP-MME vs SDS-WAS: Results 2016



DOD AERONET Direct-sun Version 3 Level 1.5 comparison

Statistics ICAP-MME Mean

	NDATA	MEAN_obs	MEAN_model	SD_obs	SD_model	COR	RMSE	MB	MNBE	MNGE	MFB	MFE
NAfrica	4137	0.43	0.43	0.36	0.33	0.79	0.22	0.00	0.08	0.37	0.02	0.38
Middle East	755	0.33	0.30	0.28	0.21	0.60	0.23	-0.04	-0.06	0.39	0.20	0.67
Mediterranean	4932	0.09	0.10	0.15	0.14	0.85	0.08	0.01	-0.14	0.43	1.04	1.39
all_selected_sites	10016	0.25	0.25	0.31	0.29	0.85	0.17	0.00	0.00	0.39	0.55	0.91

Statistics SDS-WAS Mean

	NDATA	MEAN_obs	MEAN_model	SD_obs	SD_model	COR	RMSE	MB	MNBE	MNGE	MFB	MFE
NAfrica	4428	0.42	0.34	0.35	0.23	0.74	0.25	-0.08	-0.08	0.36	-0.14	0.43
Middle East	802	0.34	0.30	0.28	0.23	0.38	0.29	-0.03	-0.08	0.36	0.18	0.65
Mediterranean	5279	0.09	0.08	0.15	0.12	0.84	0.08	0.00	-0.27	0.46	0.99	1.44
all_selected_sites	10716	0.24	0.20	0.31	0.22	0.80	0.19	-0.04	-0.14	0.39	0.45	0.96

Statistics SDS-WAS Median

	NDATA	MEAN_obs	MEAN_model	SD_obs	SD_model	COR	RMSE	MB	MNBE	MNGE	MFB	MFE
NAfrica	4440	0.42	0.31	0.35	0.20	0.79	0.26	-0.12	-0.20	0.36	-0.27	0.48
Middle East	809	0.33	0.26	0.28	0.14	0.64	0.23	-0.08	-0.19	0.35	0.09	0.68
Mediterranean	5293	0.09	0.07	0.15	0.11	0.86	0.08	-0.02	-0.38	0.50	0.91	1.49
all_selected_sites	10750	0.24	0.18	0.31	0.19	0.85	0.19	-0.06	-0.26	0.40	0.35	1.01

Near future Operational Updates



CURRENT FORECASTING – DEVELOPED/AVAILABLE – UNDER DEVELOPMENT - PLANNED

DOMAIN	GLOBAL (ICAP)
Model	MONARCH
Status	QO
Meteorology	Inline: NMMB
Resolution	1.4x1 deg 0.7x0.5 deg
levels	24 48
DA	LETKF
Assimilated Obs	MODIS DT+DB (DU) MODIS DT+DB (ALL)
Aerosol Species	DU, SS, BC, POA, SOA bio, SOA anthro, SU, NI
Gas phase chemistry	CBM-IV CB05 ONLINE and CLIMATOLOGY
Emissions	HERMES 3.0 (HTAP v2) MEGAN ONLINE
Bio. Burn. Emissions	GFAS NRT

2017: New Marenostrum up in July
Full model into ICAP ensemble

Scalability tests and setting final resolution

Further tuning of
- emissions by region,
- wet scavenging
- optical properties

2018 Q2: Data assimilation with full aerosol model
Autosubmit workflow

Regional forecasts for Europe and Spain