ResearchConcepts Io

From Air Pollution to Climate Change - Model Evaluation Results Featuring EQSAM4clim

Swen Metzger
ResearchConcepts io GmbH
Freiburg i.Br., Germany

9th Annual EMAC Symposium
Forschungszentrum Jülich

July 03, 2019

EQSAM4clim – Important improvements over EQSAM
EQSAM is widely used as core of many aerosol models

Model Features	EQSAM4clim	EQSAM
Aerosol equilibrium partitioning model	YES	YES
(full & numerical efficient gas-liquid-solid aerosol partitioning)	(improved treatment)	(simplified treatment)
Activity coefficient parameterization	YES	YES
(water activity expressed as function of relative humidity)	(Metzger et al., 2012)	(Metzger et al., 1999)
Analytical solver (no iterative root finding)	YES	YES
(computationally very efficient & free of numerical noise)	(Metzger et al., 2016)	(Metzger et al., 2002a,b)
Explicit aerosol hygroscopic growth	YES	NO
(salt compounds based on neuztalization of cations and anions)	(Metzger et al., 2012, 2016)	simplified (Metzger 2000)
Consistent inclusion of major mineral cations	YES	NO
(NH_3/NH_4^+,HNO_3/NO_3^-,HCl/Cl^-, $H_2SO_4/HSO_4^-/SO_4^{2-}$,	(Cations/Anions)	(simplified treatment)
Ca^{2+},Mg^{2+},K^+,Na^+,H_2O–system)	(Metzger et al., 2016)	(Metzger et al., 2006)
Unique single solute parameter approach	YES	NO
(improved water uptake of mixed particles (RHD/MRHD)	(Metzger et al., 2012, 2016)	simplified (Metzger 2000)
Water uptake from nano-particles up to CCN	YES	NO
(metastable aerosols, hysteresis, Kelvin-term, Köhler curve)	(Metzger et al., 2016, 2018)	

EQSAM worldwide applications

EMAC/GMXe/MADE3 – Climate modelling applications

(e.g., Table 1 of Metzger et al., 2018, https://doi.org/10.5194/acp-18-16747-2018)

Climate and mesoscale applications

(e.g., U.S. NASA/GISS GCM, French Meso-NH, Spanish NMMB/BSC-CTM, and many more)

ECMWF C-IFS – Air pollution modelling applications

C-IFS PM2.5 ensemble forecasts are based on EQSAM (Flemming et al., 2015).
C-IFS PM2.5 ensemble forecasts are used by e.g., DWD, Meteoblue AG, Windy ...
Upgrade to EQSAM4clim foreseen (pers. comm.)

EMEP/MSC-W – Air pollution modelling Europe

EQSAM (e.g., Tsyro, 2005), EQSAM4clim part of EMEP report 2019 (pers. comm.)

CAMx – Air pollution modelling U.S. (and worldwide)

EQSAM4clim (e.g., Koo et al., 2018)

Comprehensive Air quality Model with extensions (CAMx) community model, maintained in the U.S. by G. Yarwood et al., Ramboll Environ (http://www.camx.com)

It's part of the Danish Ramboll Group, a leading engineering, design and consultancy company founded in Denmark in 1945 (with 15,000 employees, 300 offices, 1.4 billion euro, https://ramboll.com).

CAMx has been used in more than 20 countries on nearly every continent

CAMx has been employed extensively by local, state, regional, and federal government agencies, academic and research institutions, and private consultants for regulatory assessments and general research throughout the U.S. and the world

ITM presentation, 14 - 18 May 2018 – introducing EQSAM4clim option

36th International Technical Meeting on Air Pollution Modelling and its Application

RAMBOLL

RC ResearchConcepts io

Comparing the ISORROPIA and EQSAM Aerosol Thermodynamic Options in CAMx

Bonyoung Koo[1*], Swen Metzger[2*], Pradeepa Vennam[1], Chris Emery[1], Gary Wilson[1], and Greg Yarwood[1]

[1] Ramboll, 773 San Marin Drive, Suite 2115, Novato, CA 94945, USA (www.ramboll.com)
[2] ResearchConcepts io GmbH, Freiburg im Breisgau, Germany (www.researchconcepts.io)
[*] bkoo@ramboll.com; swen.metzger@eco-serve.de

Figure: *http://www.eco-serve.de/en/Data/36_ITM_Greg_Yarwood_70_poster_final_REV.pdf*

Model Prediction of PM2.5 Components

Monthly Average Concentrations of Nitrate and Ammonium (January)

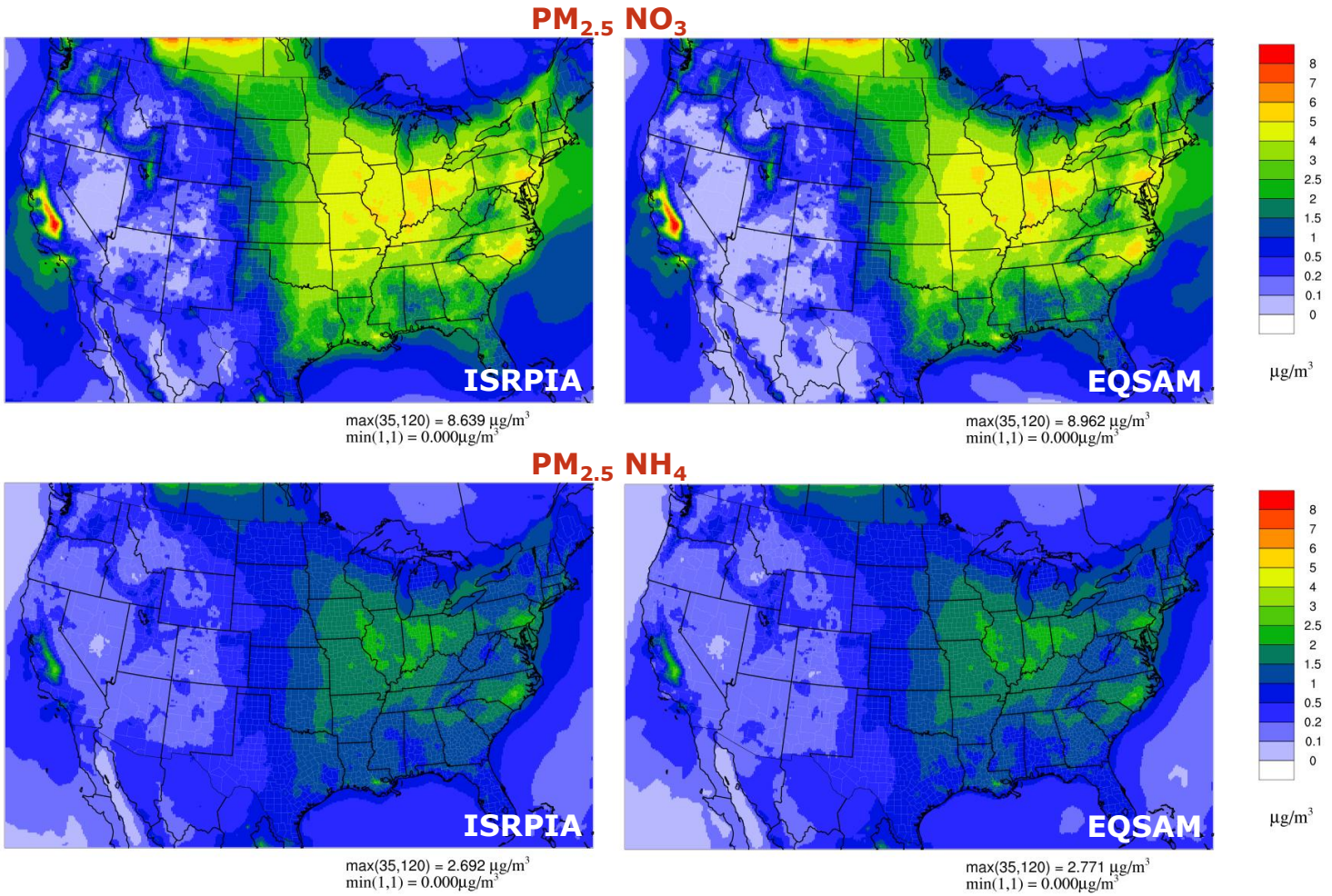


Figure: *Koo et al., ITM 2018 Presentation: 36th International Technical Meeting on Air Pollution Modelling and its Application, 14 - 18 May 2018, The Lord Elgin Hotel, Ottawa, Canada, (In conjunction with the Annual WMO-GURME Meeting).*

Model Prediction of New Source Impact

Maximum Impacts on 24-h Nitrate and Ammonium (January)

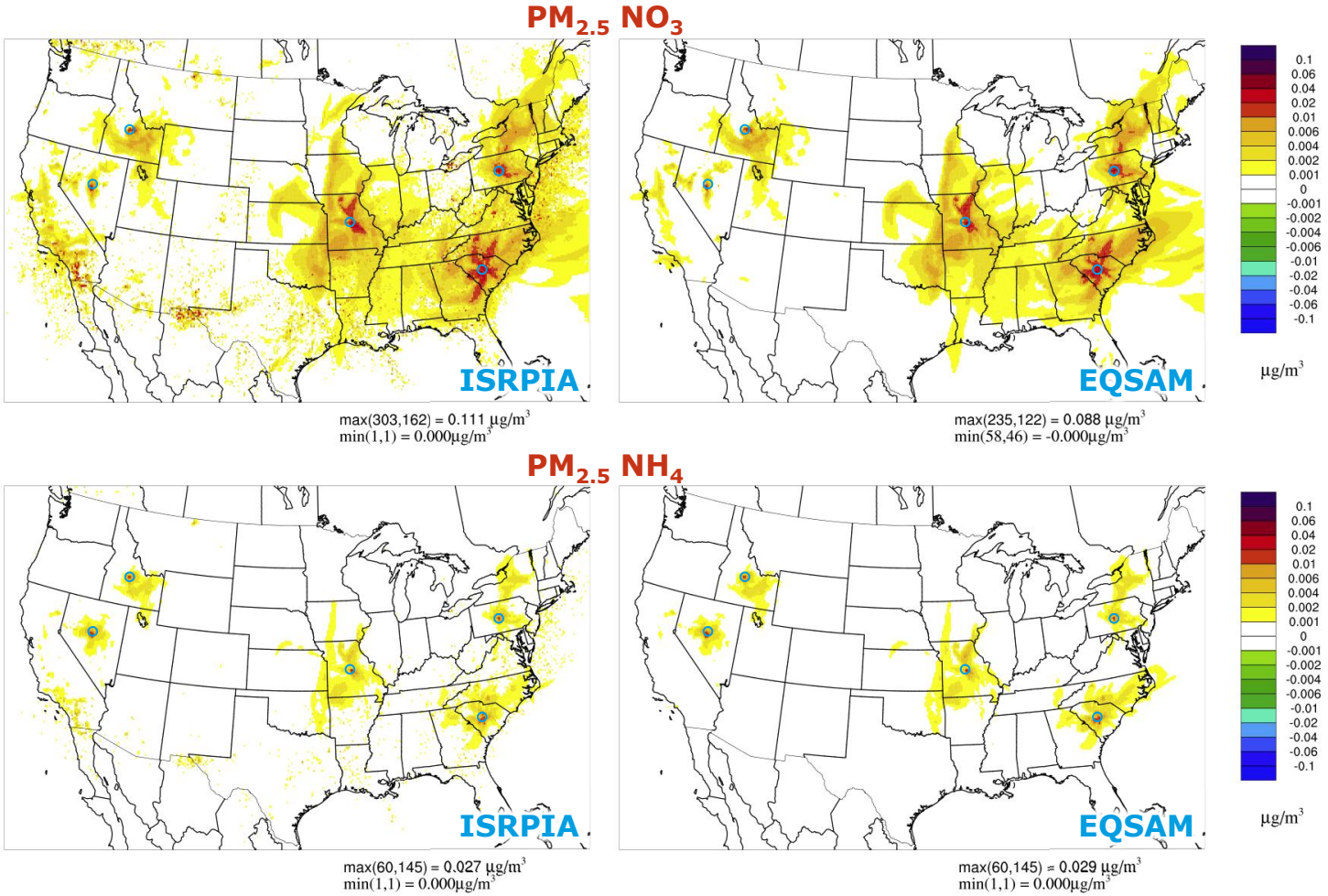


Figure: *Koo et al., ITM 2018 Presentation: 36th International Technical Meeting on Air Pollution Modelling and its Application, 14 - 18 May 2018, The Lord Elgin Hotel, Ottawa, Canada, (In conjunction with the Annual WMO-GURME Meeting).*

Numerical Artifacts of ISORROPIA

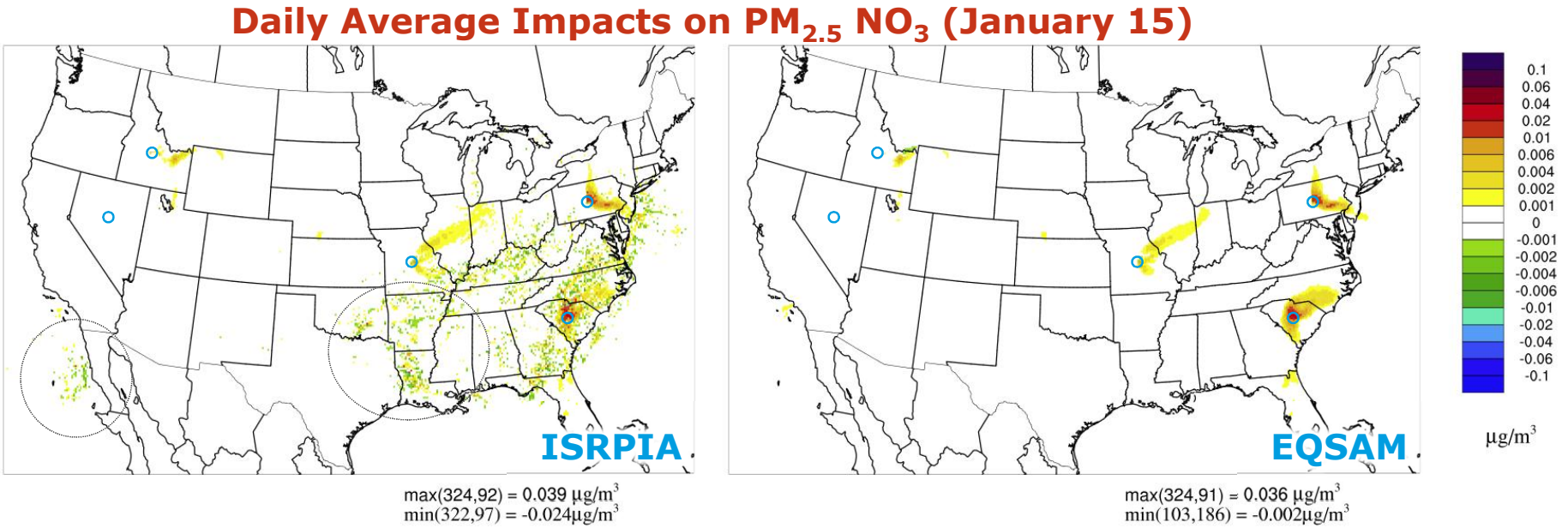


Figure: *Koo et al., ITM 2018 Presentation: 36th International Technical Meeting on Air Pollution Modelling and its Application, 14 - 18 May 2018, The Lord Elgin Hotel, Ottawa, Canada, (In conjunction with the Annual WMO-GURME Meeting).*

Short Summary A computationally efficient thermodynamic equilibrium model, EQSAM4clim was implemented in CAMx and compared with ISORROPIA. Both models? results are sufficiently similar that either could reasonably be selected. Advantages of using EQSAM are that it runs faster (in our test, EQSAM reduced the overall CAMx runtime by 4% (January) to 7% (July)) relative to the overall CPU usage of CAMx. Noteworthy, EQSAM4clim is free of numerical artifacts (`http://www.eco-serve.de/en/Data/36_ITM_Greg_Yarwood_70_poster_final_REV.pdf`*).*

Overview

European Monitoring and Evaluation Programme = EMEP

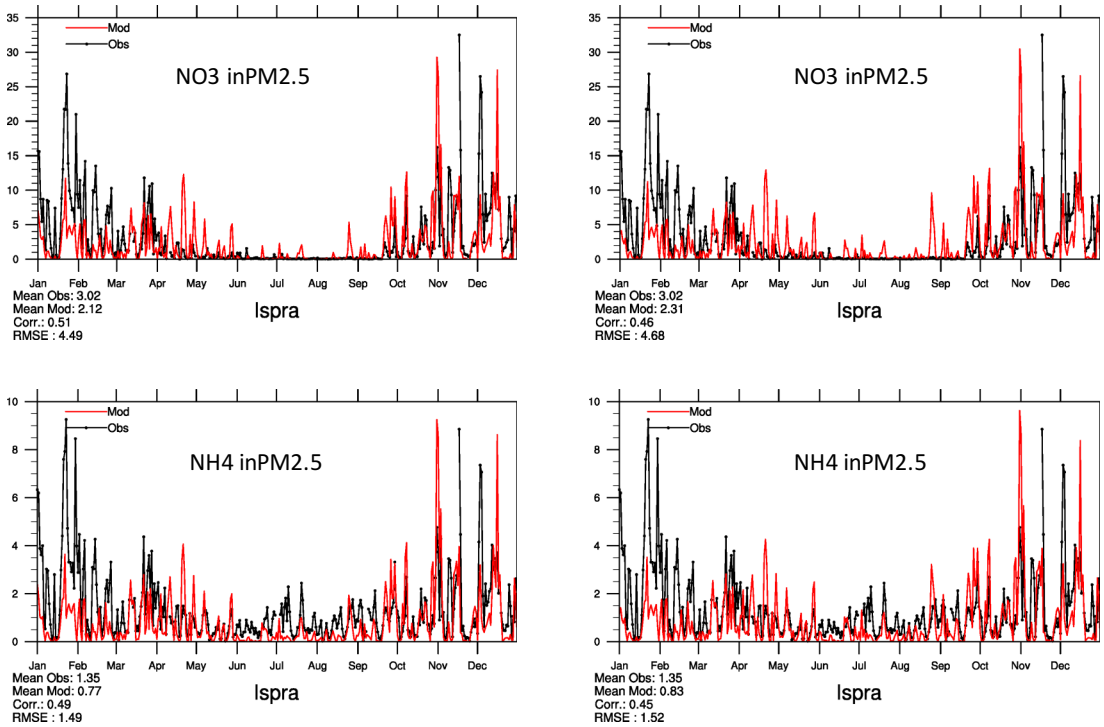
The co-operative programme for monitoring and evaluation of the long-range transmission of air pollutants in Europe (inofficially 'European Monitoring and Evaluation Programme' = EMEP) is a scientifically based and policy driven programme under the Convention on Long-range Transboundary Air Pollution (CLRTAP) for international co-operation to solve transboundary air pollution problems.

Five EMEP Centers and four Task Forces undertake efforts in support of the EMEP work plan. Please refer to the respective websites for in-depth information: https://www.emep.int.

1. Task Force on Emission Inventories and Projections (TFEIP)
2. Task Force on Measurements and Modeling (TFMM)
3. Task Force on Integrated Assessment Modelling (TFIAM)
4. Task Force on Hemispheric Transport of Air Pollution (TFHTAP)

Aerosol fine mode ammonium and nitrate

EQSAM4clim **MARS**



Norwegian Meteorological Institute

Figure: *Recent EMEP MSC-W model developments to improve secondary inorganic aerosols, Presented by Svetlana Tsyro, TFMM 20-th meeting Madrid, May 7-9, 2019.*

EMEP Task Force on Measurements and Modelling (TFMM), https://projects.nilu.no//ccc/tfmm/index.html, https://projects.nilu.no//ccc/tfmm/madrid_2019/20190507/5_TFMM_2019_Madrid_eqsam_Tsyro.pptx

Aerosol fine mode nitrate (selected stations)

NO_3^- in $PM_{2.5}$

	OBS	eq4cl	mars	R eq4cl	R mars
DE01	**1.99**	**2.25**	2.44	**0.39**	0.34
DE02	**2.48**	**2.95**	3.13	**0.49**	0.46
DE08	**1.58**	**2.50**	2.69	**0.41**	0.37
FR09	**1.81**	**2.88**	2.97	**0.23**	0.20
FR24	**1.57**	**2.33**	2.44	**0.46**	0.46
SI08	**0.31**	**0.93**	0.93	**0.49**	0.48

Similarly, some improvement is found for NH_4^+ in $PM_{2.5}$

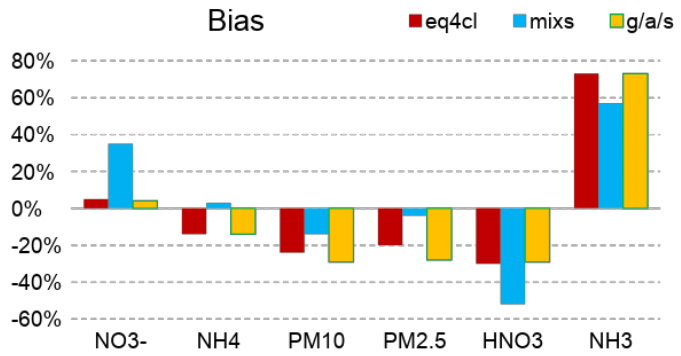
Norwegian Meteorological Institute

Figure: *Recent EMEP MSC-W model developments to improve secondary inorganic aerosols, Presented by Svetlana Tsyro, TFMM 20-th meeting Madrid, May 7-9, 2019.*

EMEP Task Force on Measurements and Modelling (TFMM), https://projects.nilu.no//ccc/tfmm/index.html, https://projects.nilu.no//ccc/tfmm/madrid_2019/20190507/5_TFMM_2019_Madrid_eqsam_Tsyro.pptx

Modeling Options

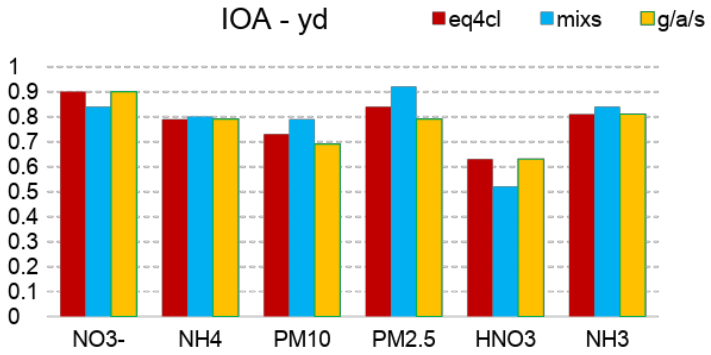
EQSAM4clim: testing setups



EQSAM4clim allows flexibility wrt included processes and gas/aerosol components (cations and anions) and variable degree of complexity..

Ideally, all major cation/anions should be included for best result

Presently, base cations from mineral dust are not accounted for



eq4cl – metastable aqueous aerosols, gas/aerosol partitioning (as in MARS)

mixs – equil. dissociation constant Kp for NH_4NO_3 not only f(RH, T), but also f(composition): decreases with increasing $(NH_4)_2SO_4$) content

g/a/s – full gas/aerosol/solid equilibrium

Norwegian Meteorological Institute

FIGURE: *Recent EMEP MSC-W model developments to improve secondary inorganic aerosols, Presented by Svetlana Tsyro, TFMM 20-th meeting Madrid, May 7-9, 2019.*

EMEP Task Force on Measurements and Modelling (TFMM), https://projects.nilu.no//ccc/tfmm/index.html, https://projects.nilu.no//ccc/tfmm/madrid_2019/20190507/5_TFMM_2019_Madrid_eqsam_Tsyro.pptx

Overview

European Organisation for the Exploitation of Meteorological Satellites = EUMETSAT

EUMETSAT has released in January 2016 the Polar Multi-sensor Aerosol product version 2.1 (PMAp2). Further info is available at: `http://www.eco-serve.de/en/Results.html`.

EUMETSAT ITT 15/210839

We have evaluated the Polar Multi-sensor Aerosol product version 2 (PMAp2) of the Meterological Operational Satellites (MetOp) A and B on global scale using MISR-Terra, MODIS-Aqua/Terra, AERONET, CASTNET, EMEP and EMAC data. Our cross-platform analysis comparison based on a 0.5 hour temporal collocation window and a 30 km radius for the spatial collocation relative to AERONET station observations, and a fairly high spatial (0.1 by 0.1) and high temporal model resolution (hourly output globally), reveals best the differences and similarities between the various AOD products, which are most likely caused by various cloud masking assumptions. For PMAp2.1, AERONET and EMAC, the best agreement is found for the Caribbean, NE America, European and Asian stations, while generally, the PMAp2 AOD time-series are supported by our model result, which are mostly in good agreement with independent AOD (AERONET, MODIS, MISR), and aerosol composition (CASTNET, EMEP) observations (Final Acceptance Review (FAR) presentation: `https://bit.ly/2QObx8V`).

PMAp2 Evaluation – EUMETSAT ITT 15/210839

We use an augmented version of the EMAC Model

Metzger et al., 2016, Aerosol Water Parameterization: A single parameter framework
Abdelkader et al., 2015, Dust–air pollution dynamics over the eastern Mediterranean
Abdelkader et al., 2017, Sensitivity of transatlantic dust transport to chemical aging and related atmospheric processes

The EMAC Earth-System Model is a community modelling effort: http://www.messy-interface.org

with our augmented version being an outcome of the cooperation of the Max Planck Institute for Chemistry in Mainz and The Cyprus Institute.

The advantage of our EMAC version

is the detailed chemical and micro-physical processes and the high resolution simulations.

EMAC (ECHAM5/MESSy 2.5.0) base model

T255-T106 L31 ($\approx$ 55–110km globally, 31 vertical levels up to 10hPa), nudged meteorology (ECWMF), state-of-the-art anthropogenic emissions, chemical aging & water uptake, online calculation of natural sea salt and dust aerosols in feedback with meteorolgy (soil moisture).

Selected Aeronet stations

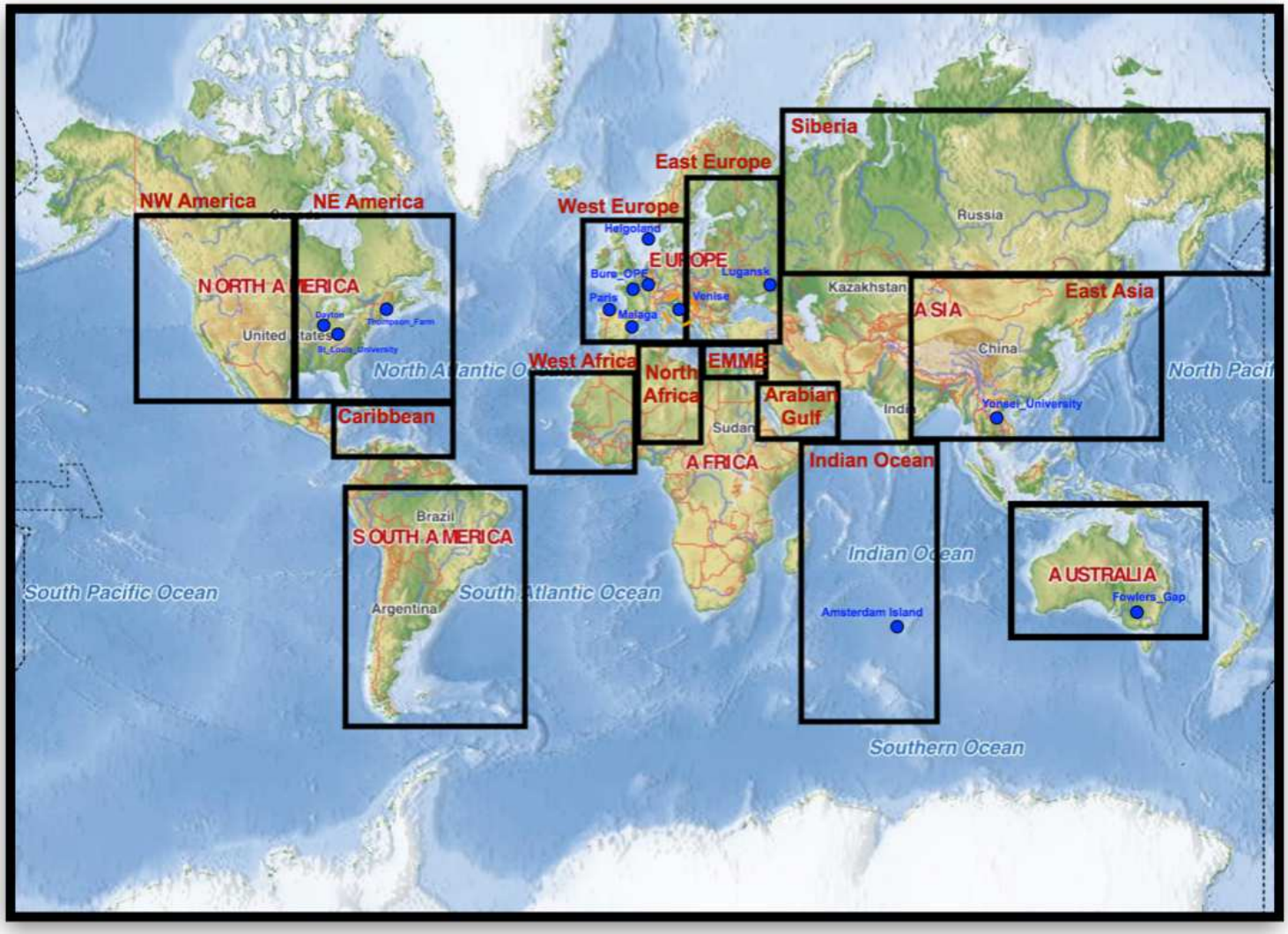


Figure: *Selected Aeronet station locations and region definition.*

1. Global (1hr avg)

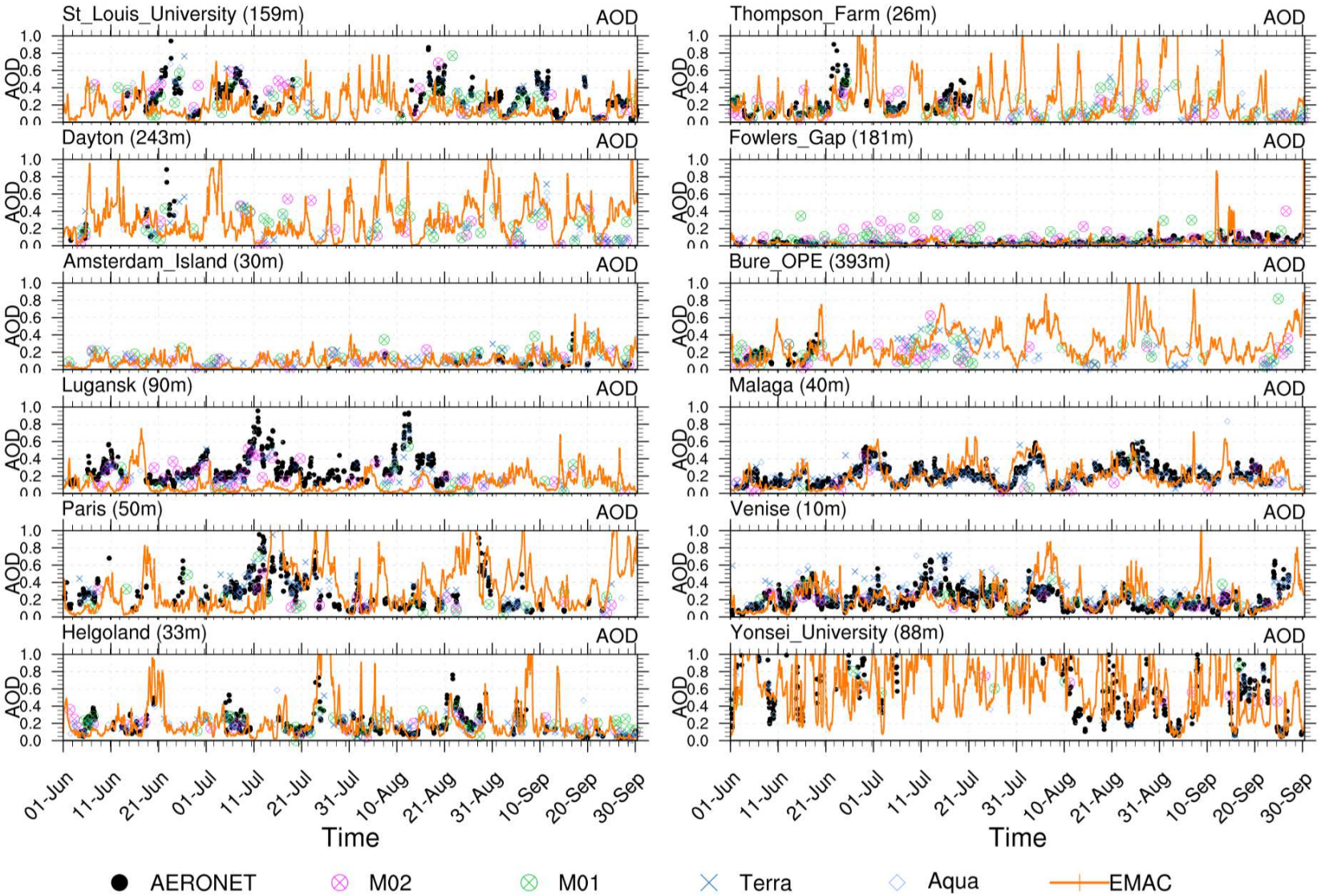


Figure: *EMAC AOD and L2 of PMAp2 (M02, M01), MODIS (Aqua, Terra), AERONET.*

2. West Europe (1hr avg)

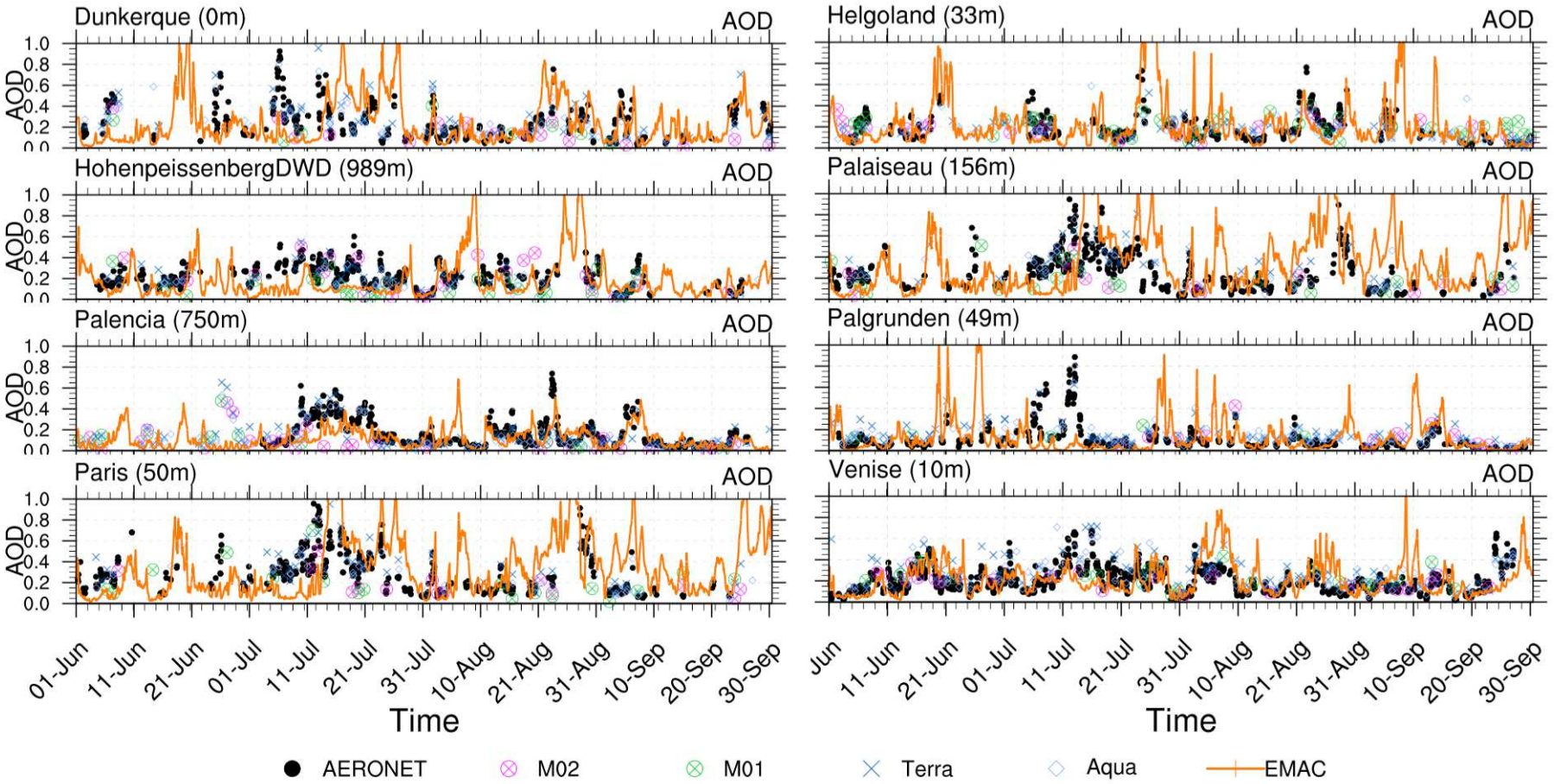


Figure: *EMAC AOD and L2 of PMAp2 (M02, M01), MODIS (Aqua, Terra), AERONET.*

3. NW America (1hr avg)

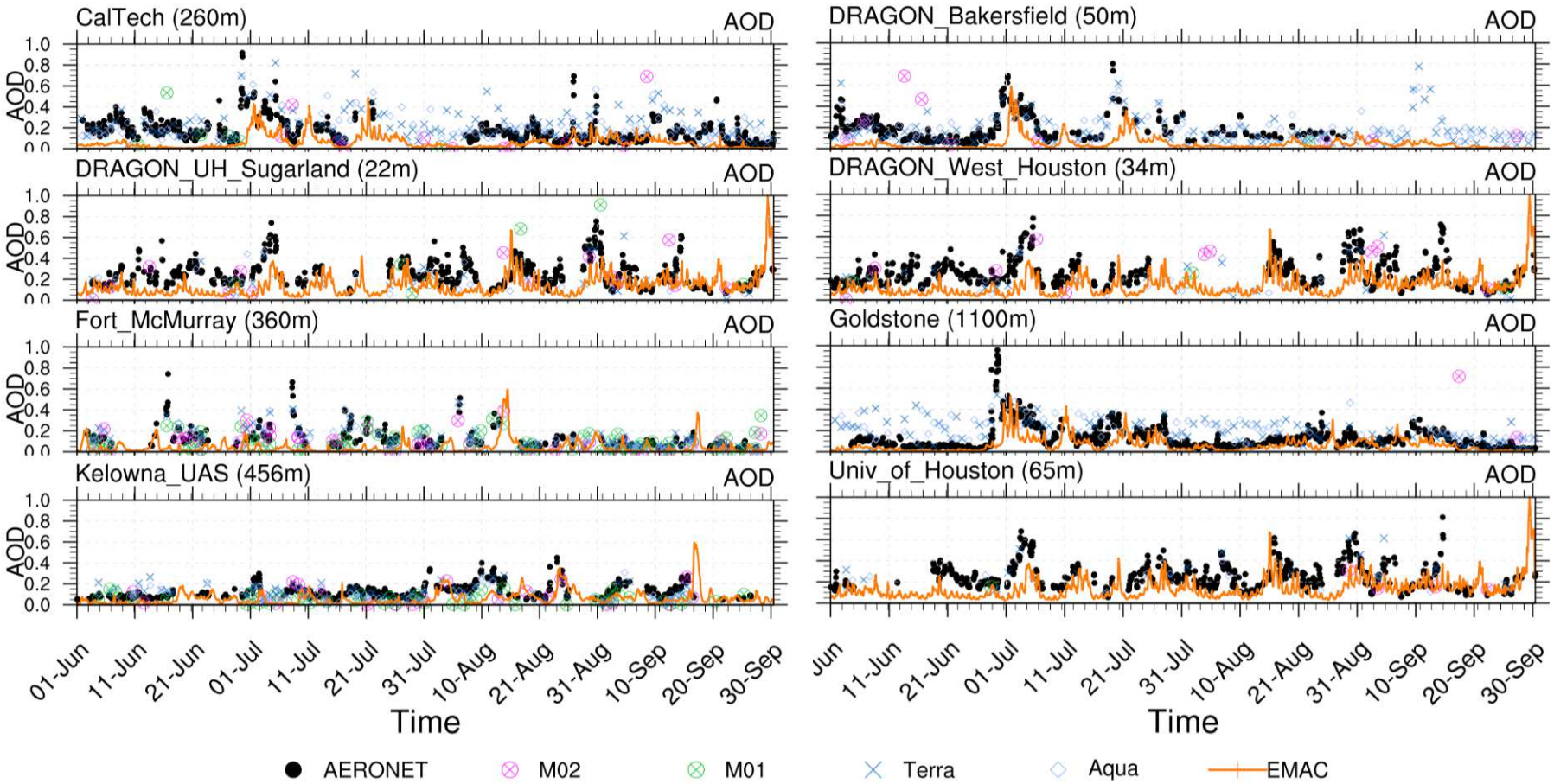


Figure: *EMAC AOD and L2 of PMAp2 (M02, M01), MODIS (Aqua, Terra), AERONET.*

4. Dust belt / outflow (1hr avg)

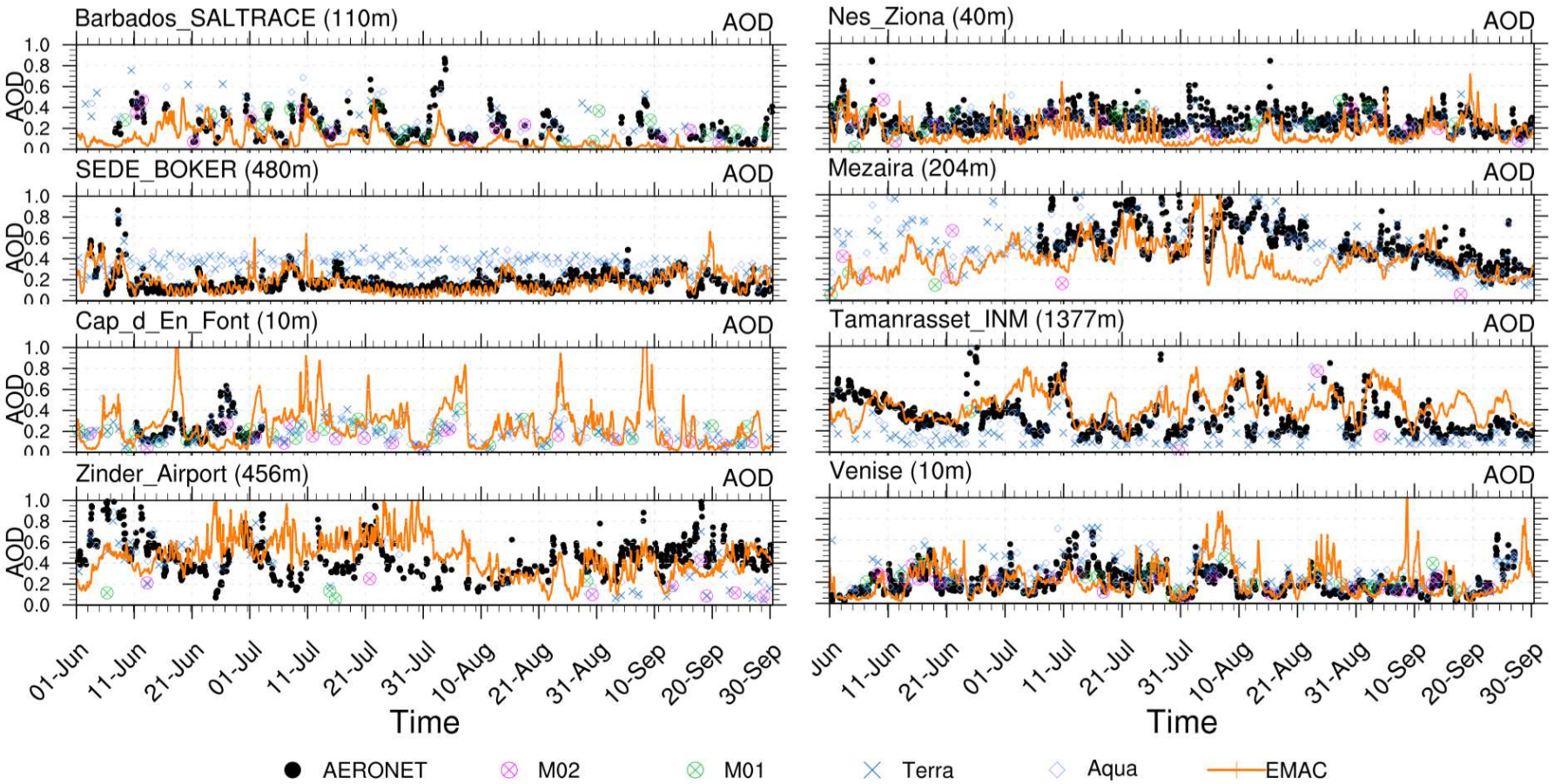


Figure: *EMAC AOD and L2 of PMAp2 (M02, M01), MODIS (Aqua, Terra), AERONET.*

EMAC modal aerosol concentrations

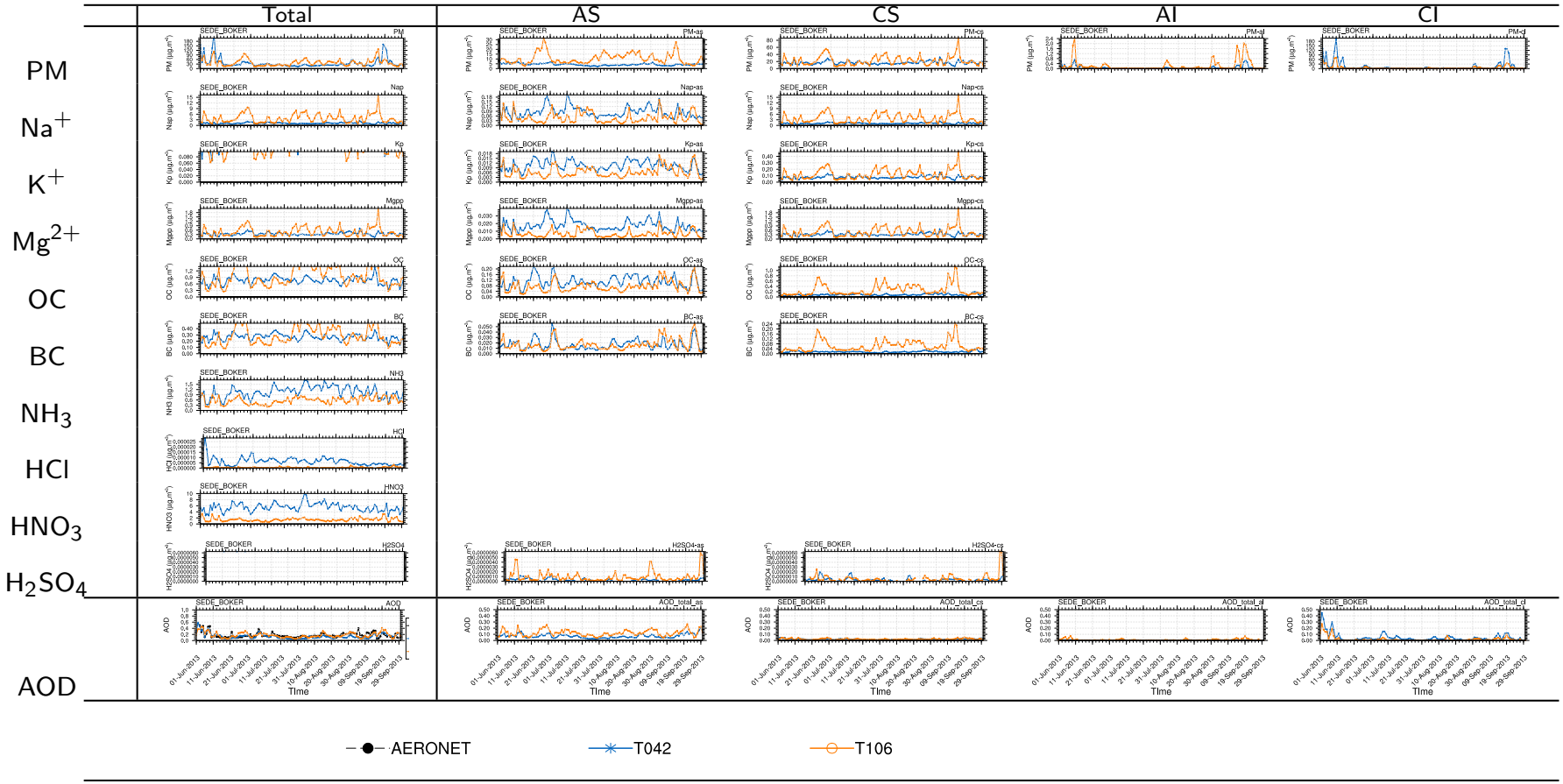


FIGURE: *Modal aerosol concentrations time series at the AERONET station Sede Boker.*

EMAC Model set-up

Model Features	EMAC(PMAp2 study)	EMAC (base version)
Online calculation of natural emissions	YES	NO
(seas spray & mineral dust)	(Abdelkader et al., 2015)	
Emission feedback with meteorology	YES	NO
(soil moisture & precipitation)	(Abdelkader et al., 2016)	
Chemical speciation of natural emissions	YES	NO
(e.g., $Na^+, K^+, Mg^{2+}, Ca^{2+}, SO_4^{2-}, HSO_4^-, Cl^-$)	(Cations/Anions)	(Bulk: SS, DU, BC/OC)
Explicit & fast aerosol hygroscopic growth	YES	N/A
(full & numerical efficient gas-liquid-solid aerosol partitioning)	(Metzger et al., 2016,2018)	
Aerosol-cloud clover coupling	YES	N/A
(aerosol hygroscopic growth in fog-haze and thin optical clouds)	(Metzger et al., 2007)	
Consistent aerosol-cloud-radiation feedbacks	YES	Uncoupled
(driven by aerosol hygroscopic growth & water vapour uptake)	(Metzger et al., 2007,2018)	
Numerically optimized EMAC submodels	YES	NO
(computationally efficient for, e.g., day-ahead solar forecasting)	(Cumpston, Metzger, Mitsos,	
(Energy oriented Centre of Excellence (EoCoE))	EoCoE Project report, 2018)	
Output optional at local time (MetOp overpass)	YES	NO

Time-series of AOD (2000-2013)

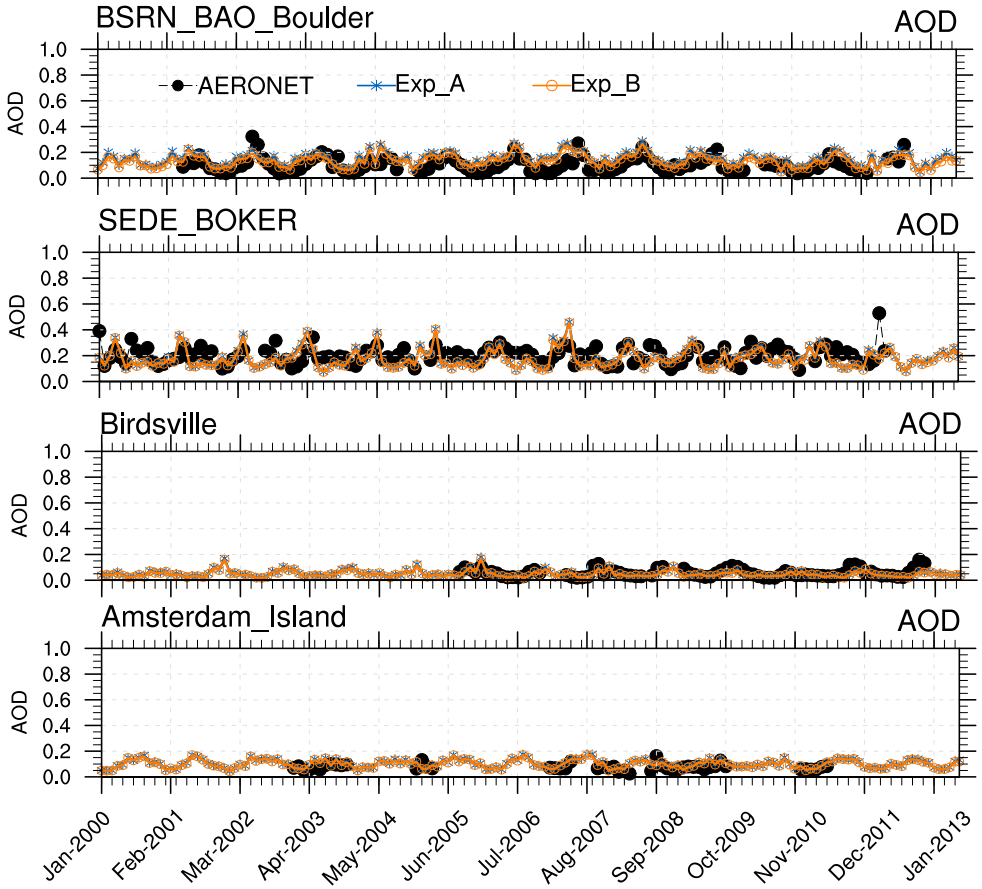
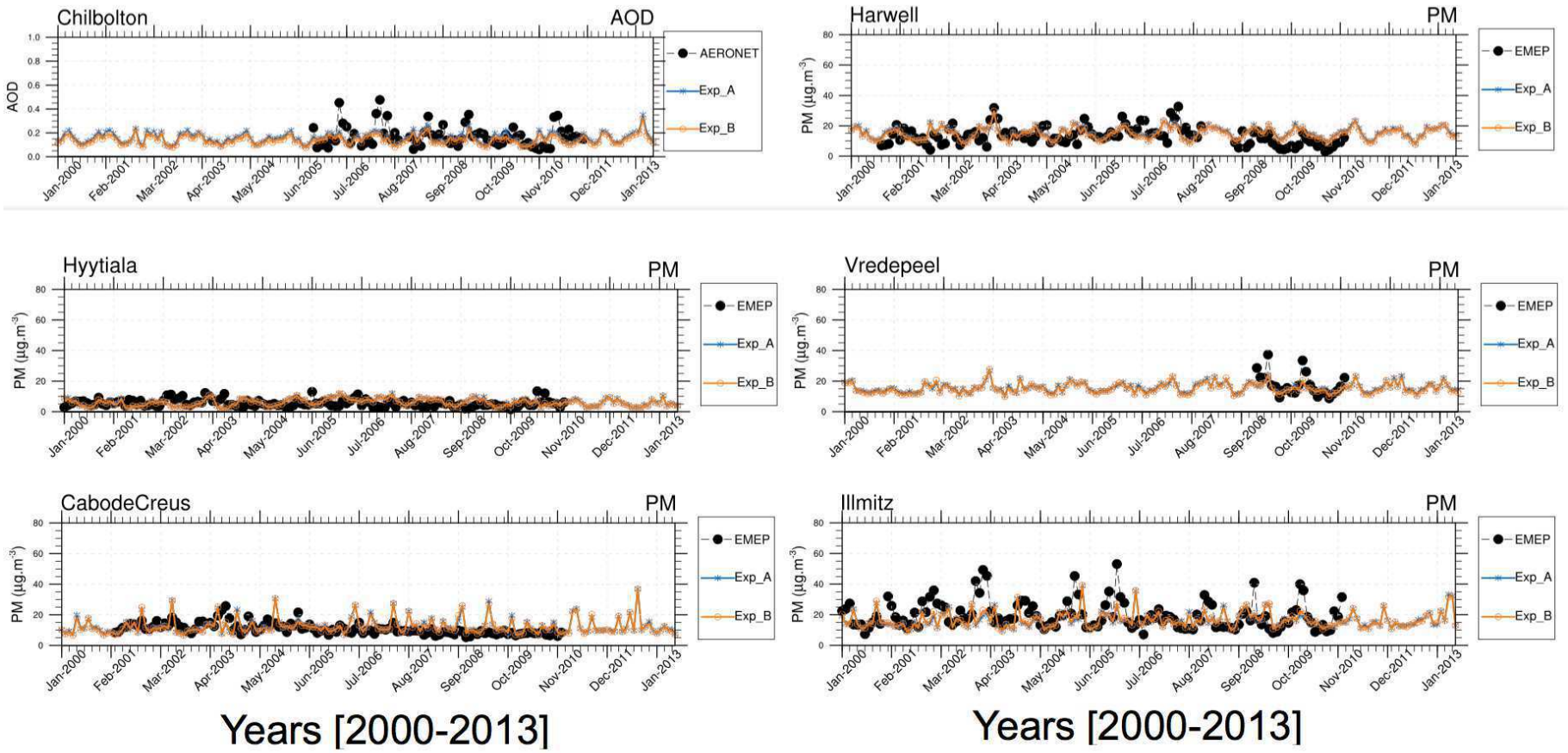


Figure: *AOD (monthly mean) at four AERONET stations that have long-term data available and which represent different aerosol types and climatic regions. AERONET observations (black line), EMAC - Exp A (ISORROPIA II, blue line), Exp B (EQSAM4clim, orange line);* `http://aeronet.gsfc.nasa.gov/cgi-bin/type_piece_of_map_opera_v2_new`.

Time-series of PM (2000-2013)



Exp A = ISORROPIA II (Fountoukis, C. and Nenes, https://doi.org/10.5194/acp-7-4639-2007)

Exp B = EQSAM4clim (Metzger et al., https://doi.org/10.5194/acp-16-7213-2016)

Figure: *EMAC aerosol particulate matter (PM) (liquid+solid aerosol compounds) at EMEP stations that have available long-term data (`http://ebas.nilu.no/default.aspx`).*

Time-series of major anions (2000-2013)

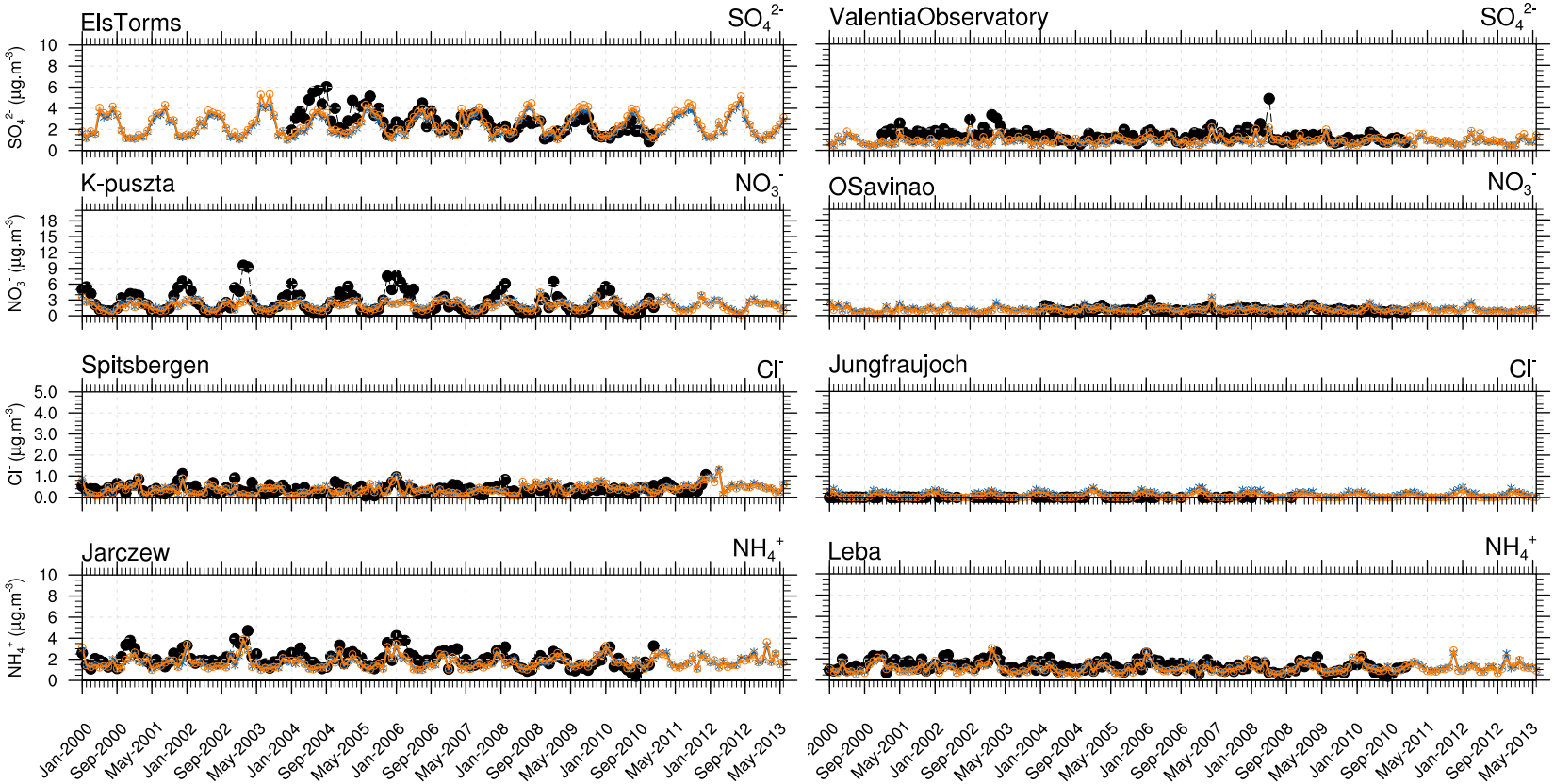


Figure: *Lumped aerosol concentrations (liquids+solids) of the EMAC simulations and EMEP observations: Sulfate (SO_4^{2-}), nitrate (NO_3^-), chloride (Cl^-), and cation ammonium (NH_4^+); each species is compared with two different station observations (left and right column, black lines); EMAC simulations based on two gas-liquid-solid partitioning schemes: ISORROPIA II (blue line), EQSAM4clim (orange line).*

Time-series of major cations (2000-2013)

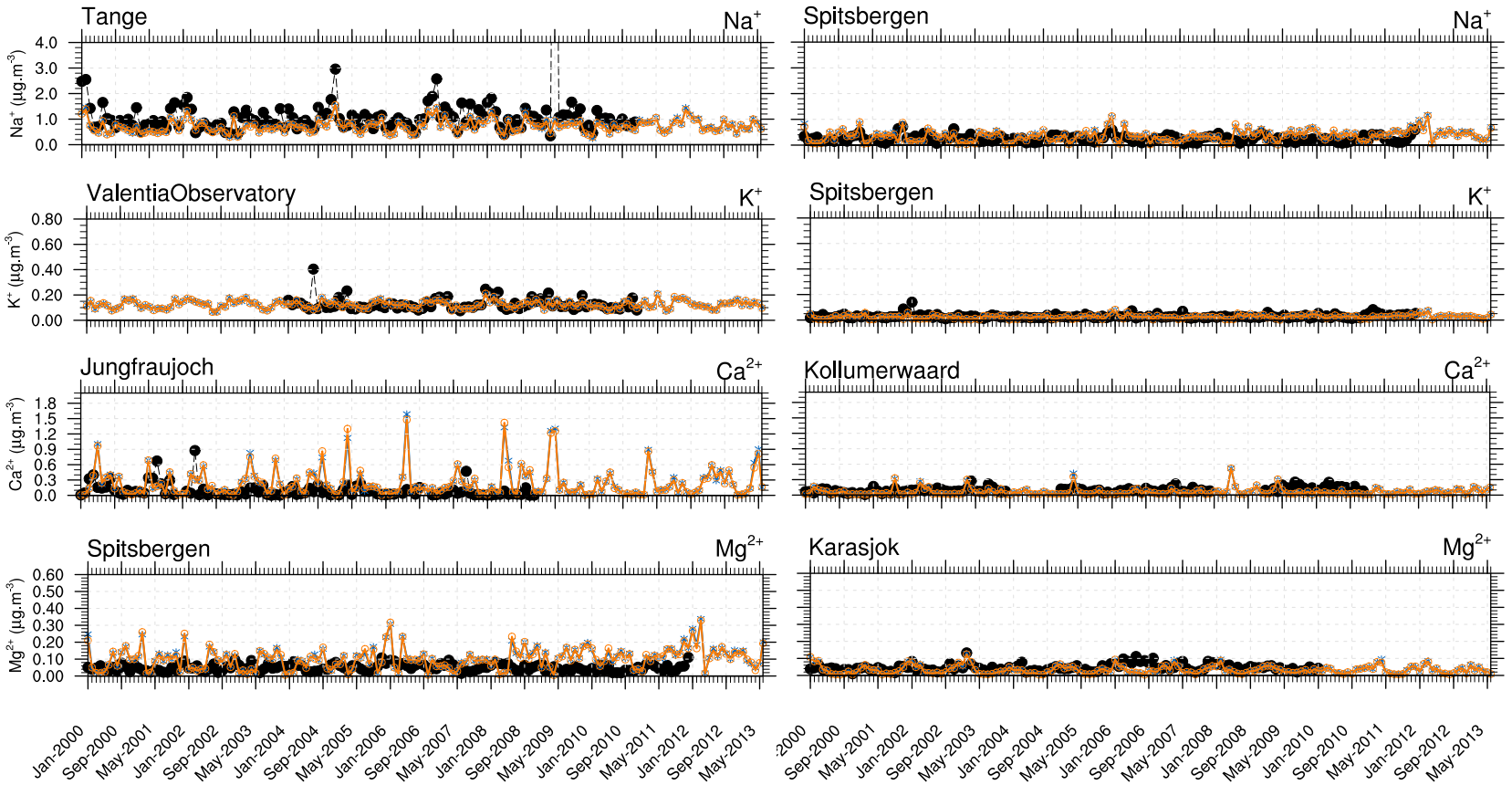


Figure: *Lumped aerosol concentrations (liquids+solids) of the EMAC simulations and EMEP observations: Sodium (Na^+), potassium (K^+), magnesium (Mg^{2+}) and calcium (Ca^{2+}); each species is compared with two different station observations (left and right column, black lines); EMAC simulations based on two gas-liquid-solid partitioning schemes: ISORROPIA II (blue line), EQSAM4clim (orange line).*

Comparison with EMEP and CASTNET observations

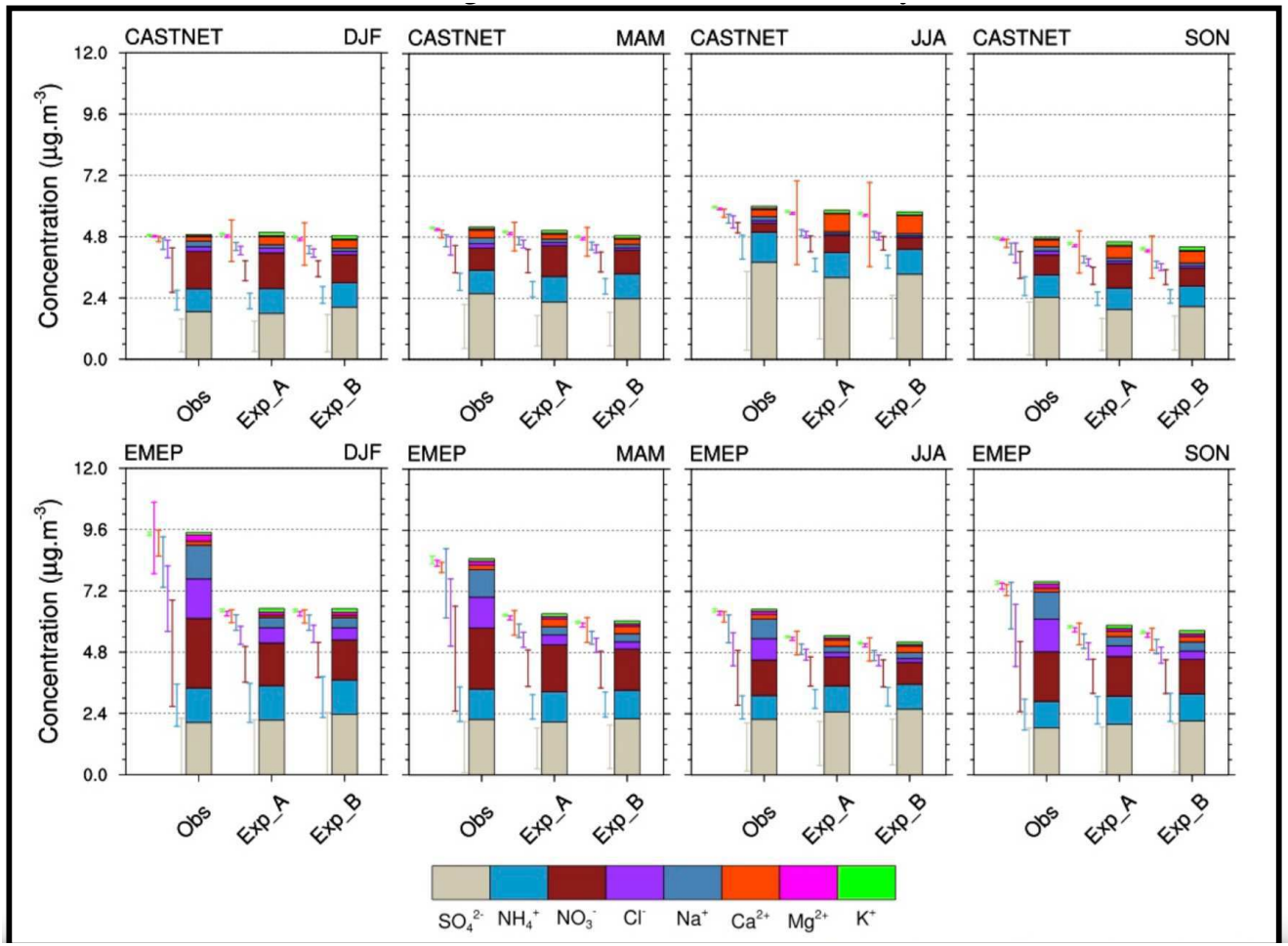


Figure: *Longterm seasonal evaluation (2000-2013) of the EMAC aerosol concentrations and composition (sulfate, ammonium, nitrate, sodium, chloride, calcium, potassium and magnesium) over Europe (EMEP) and United States (CASTNET). EMAC simulations based on two gas-liquid-solid partitioning schemes: ISORROPIA II (Exp A), EQSAM4clim (Exp B).*

EMAC aerosol water mass AOD fraction (2000-2013)

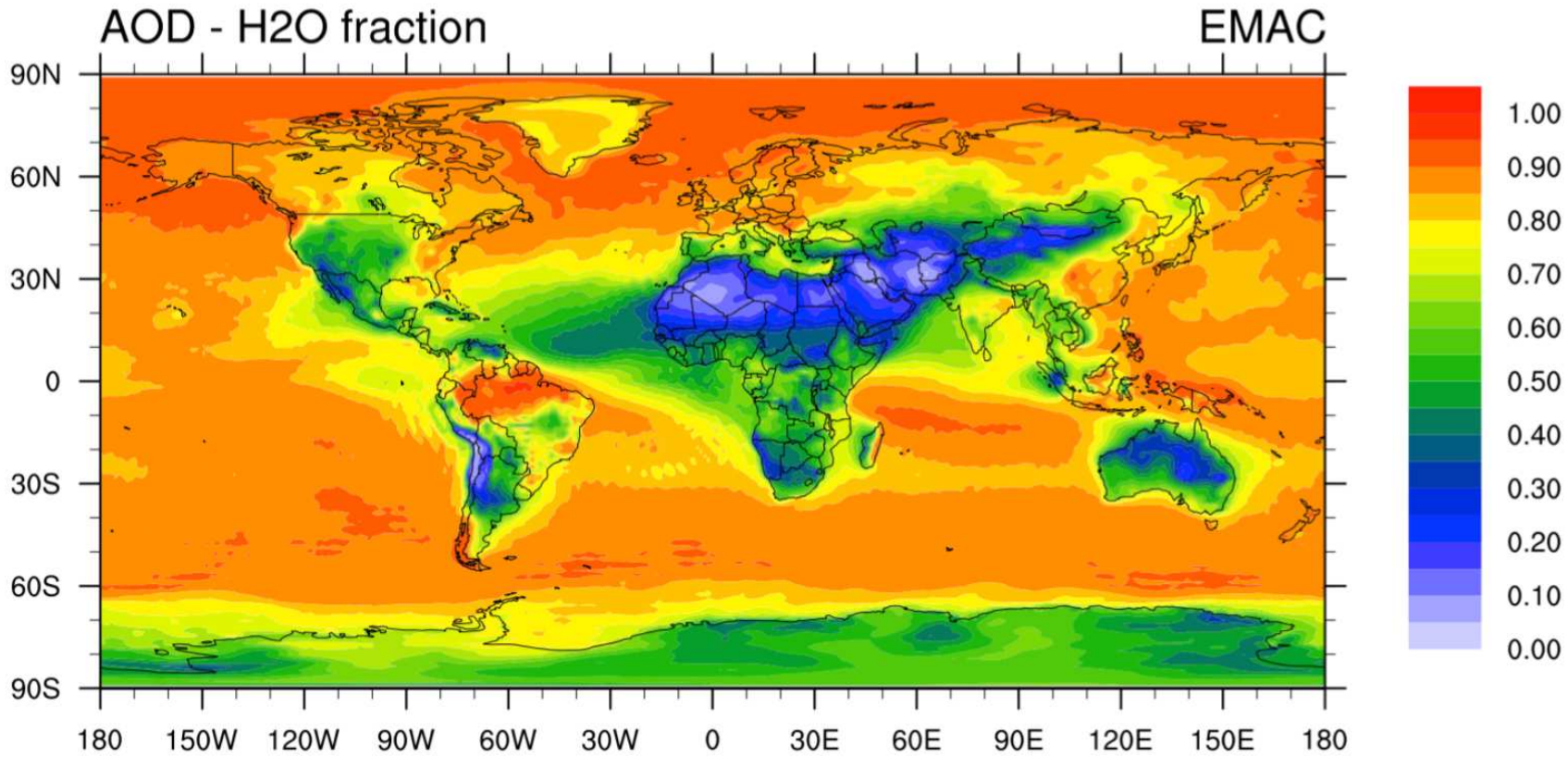


Figure: *EMAC aerosol water mass AOD fraction corresponding to the AOD distributions.*

EMAC AOD and skill score

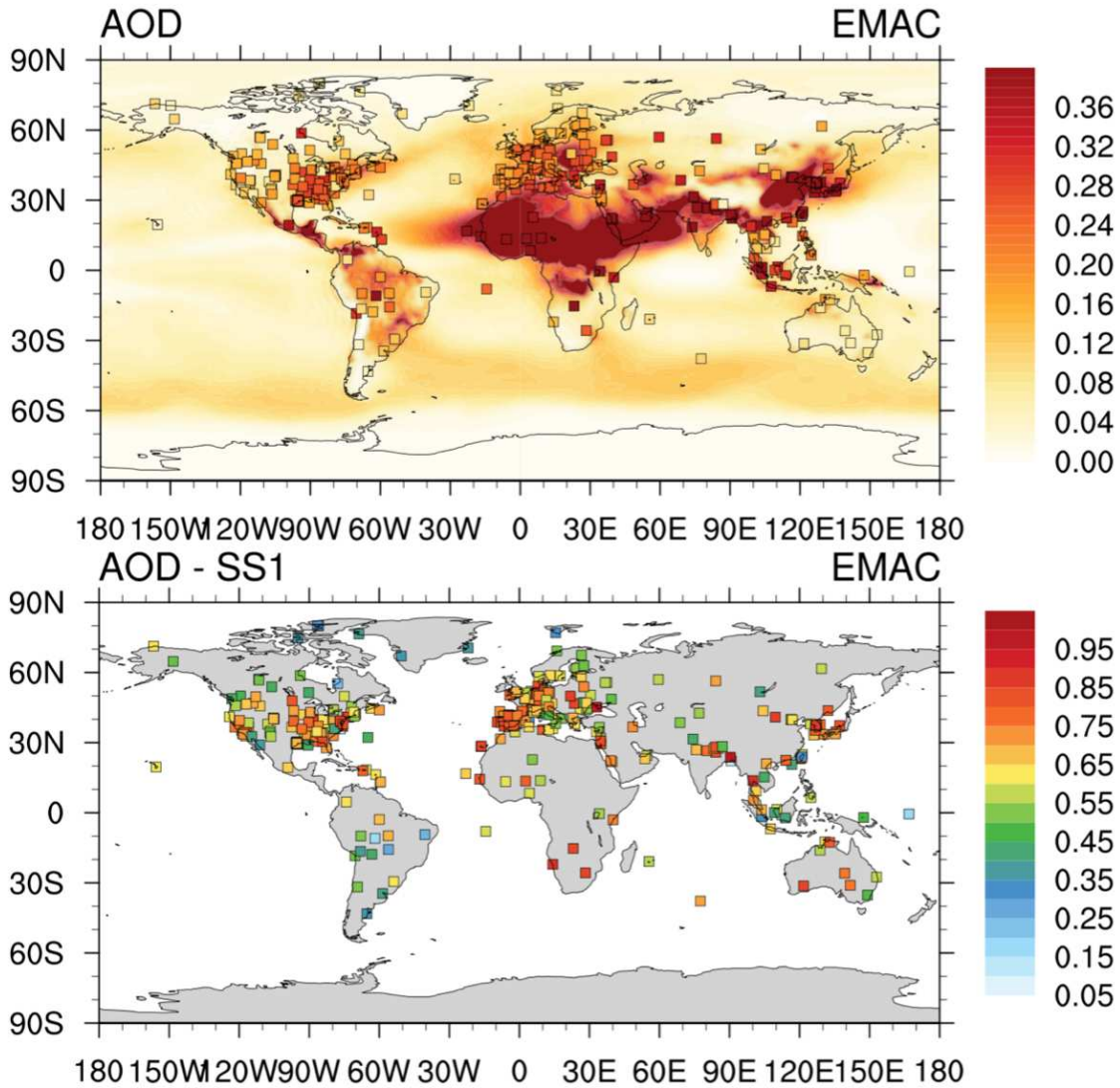


Figure: *Spacial distribution of EMAC AOD versus AERONET station observations.*

EQSAM and EQSAM4clim remain freely available

Both will be available through GitHub (https://github.com/rc-io/eqsam).

EQSAM new (old) EMAC submodel (independent of GMXe)

Complementary to GMXe, i.e., less comprehensive but numerical efficient aerosol growth calculations, size distribution similar to GM7/GMXe (submodel existed in earlier messy versions).

EQSAM4clim upgrade to EQSAM3 complexity (number of compounds)

Inclusion of major organic salt compounds and neutralization of carboxylic acids.

Ongoing development of EQSAM so far privately funded (last three years)

Users are kindly reminded to support the development, e.g., through joint projects (proposals).
Please cite the EQSAM publications in case you use it. Often EQSAM is used but not cited.

Contact the author: sm@researchconcepts.io

Visit our websites: `https://www.researchconcepts.io` and `http://www.eco-serve.de/`.

Thank you !

Selected EQSAM Publications

– Metzger et al., Gas/aerosol partitioning: 1. A computationally efficient model, JGR, https://doi.org/10.1029/2001JD001102, 2002.

– Metzger et al., Importance of mineral cations and organics in gas-aerosol partitioning of reactive nitrogen compounds: case study based on MINOS results, ACP, https://doi.org/10.5194/acp-6-2549-2006, 2006.

– Metzger et al., Reformulating atmospheric aerosol thermodynamics and hygroscopic growth into fog, haze and clouds, ACP, https://doi.org/10.5194/acp-7-3163-2007, 2007.

– Metzger et al., New representation of water activity based on a single solute specific constant to parameterize the hygroscopic growth of aerosols in atmospheric models, ACP, https://doi.org/10.5194/acp-12-5429-2012, 2012.

– Metzger et al., Aerosol Water Parameterization: A single parameter framework, ACP, https://doi.org/10.5194/acp-16-7213-2016, 2016.

– Metzger et al., Aerosol water parameterization: long-term evaluation and importance for climate studies, ACP, https://doi.org/10.5194/acp-18-16747-2018, 2018.