

Recent EMEP MSC-W model developments to improve secondary inorganic aerosols

Presented by Svetlana Tsyro

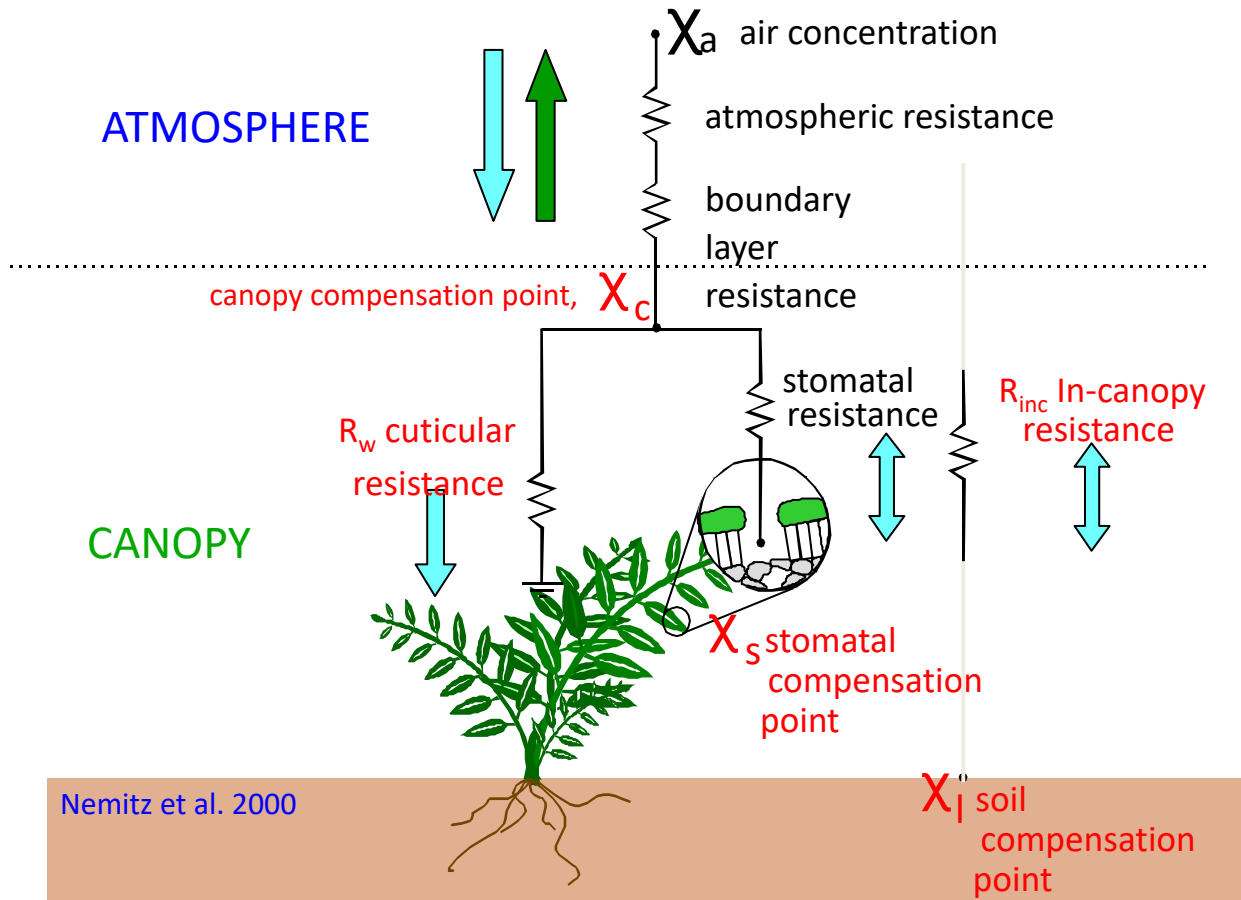
**TFMM 20-th meeting
Madrid, May 7-9, 2019**

Recent and ongoing activities (which should be) contributing to SIA improvement

- ❑ **Finer model resolution:** $0.1 \times 0.1^\circ$ and 50m lowest layer
- ❑ **Finer resolution of national emissions :** $0.1 \times 0.1^\circ$
- ❑ **Bi Directional Ammonia fluxes** (David Simpson in cooperation with TNO)
- ❑ **EQSAM4clim** - new thermodynamic equilibrium model

Bi-Directional exchange of NH_3

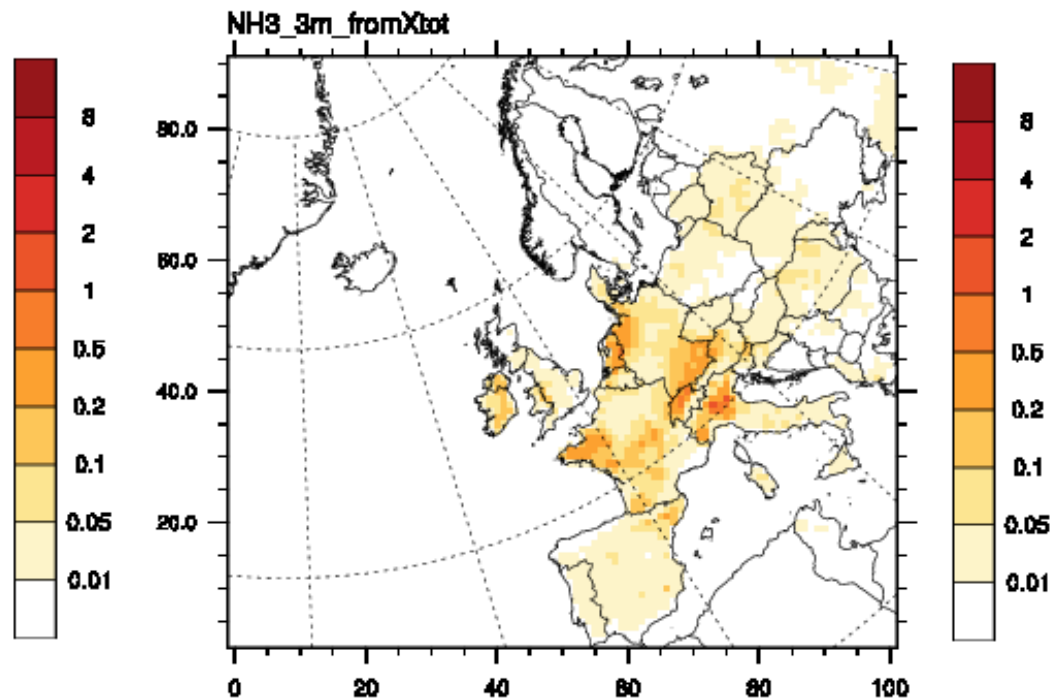
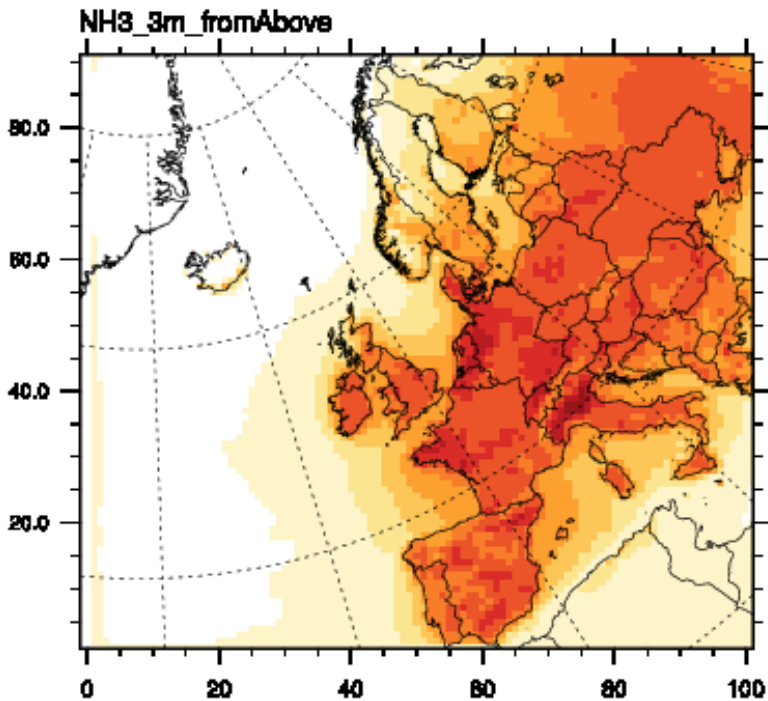
David Simpson & Roy Wichink Kruit



Towards Bi-Directional NH_3

On-going work:

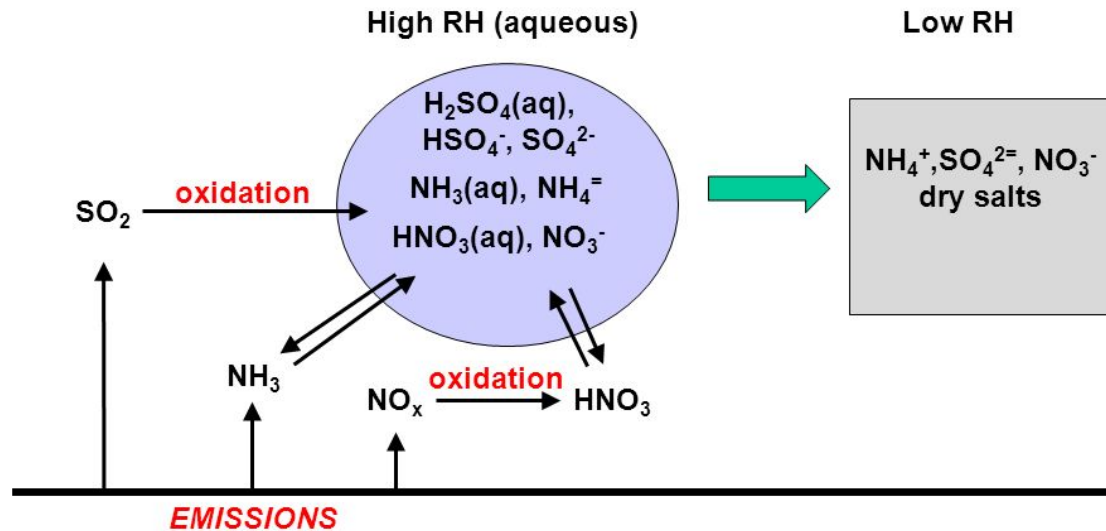
NH_3 contributions, from 'above' (left) and 'below' (right)



Courtesy of David Simpson & Roy Wichink Kruit

SIA formation & Gas-aerosol partitioning

Formation of sulfate-nitrate-ammonium (SNA) aerosol



- Uptake of NH_3 and HNO_3 by sulfate aerosol follows thermodynamics
- This uptake affects the mass and phase of the aerosol

Thermodynamic equilibrium schemes for sulphate-nitrate-ammonium-water system

«Old» EMEP scheme:

$(\text{NH}_4)_{1.5} \text{SO}_4$, simplified $K_p = f(\text{Rh}, T)$

MARS (ARES):

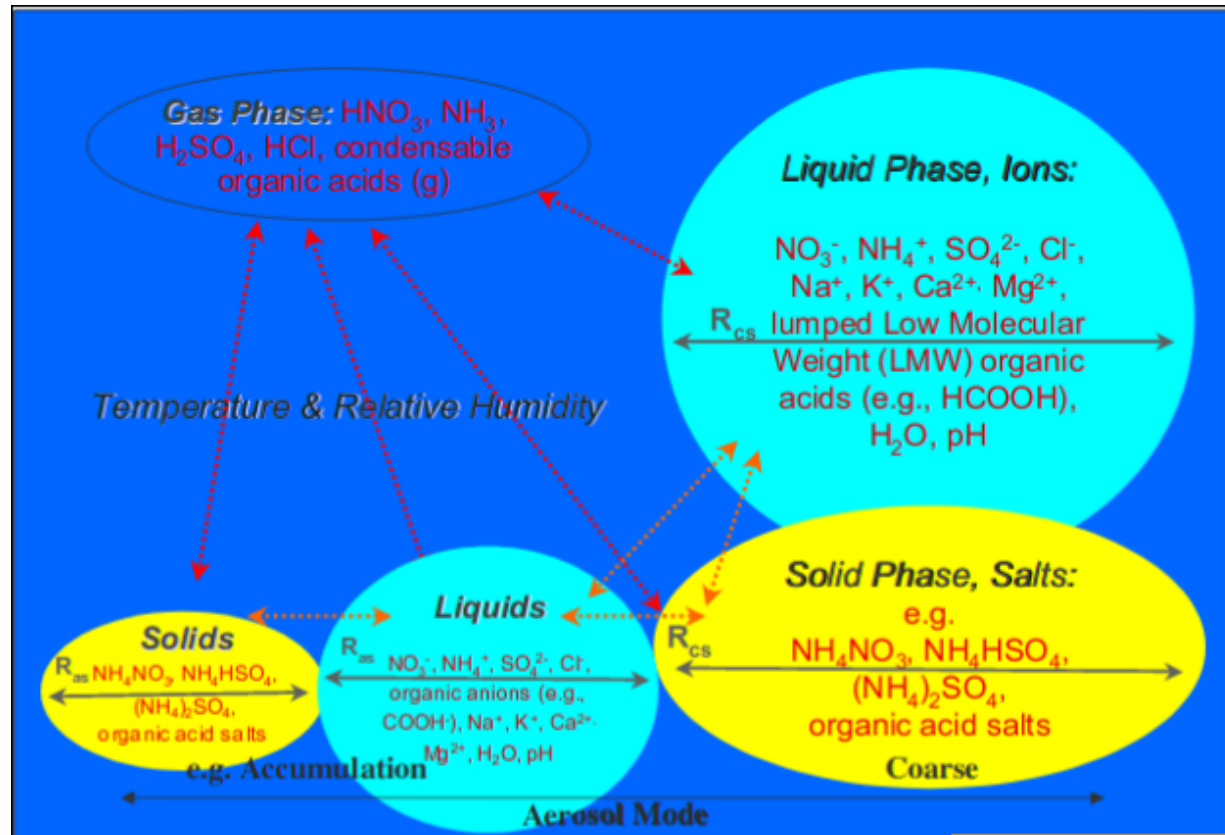
two regimes for $\text{NH}_4 / \text{SO}_4$, metastable aqueous aerosol

EQSAM-3:

parameterized version of ISORROPIA

EQSAM4clim:

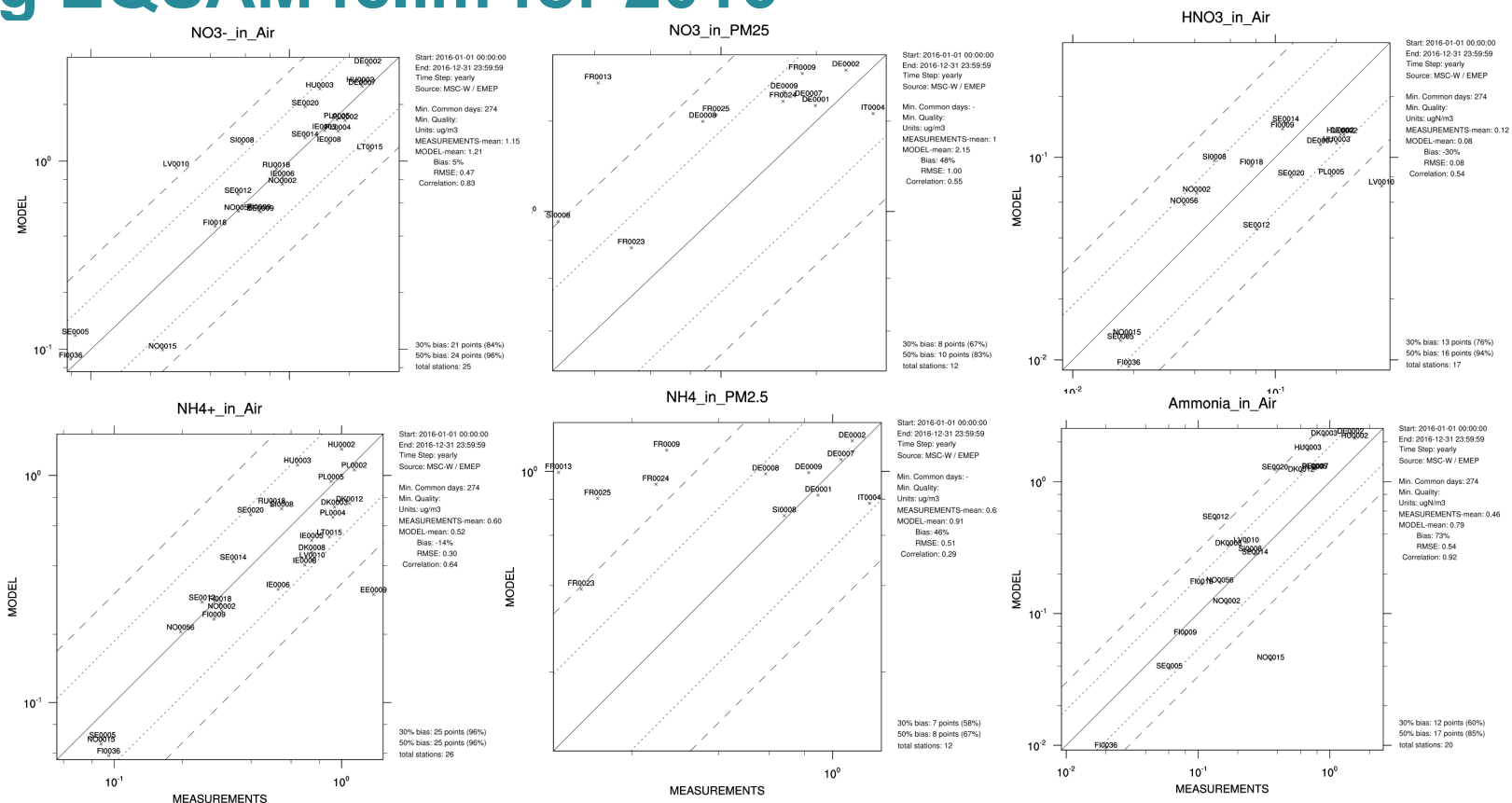
most recent version



Implemented in the EMEP MSC-W model, in close cooperation with Swen Metzger (www.researchconcepts.io, www.eco-serve.de)

Thoroughly compared against ISORROPIA, evaluated with in-situ and satellite observations (AOD) on global scale (Metzger et al., ACP (2018, 2016, 2012, 2006)

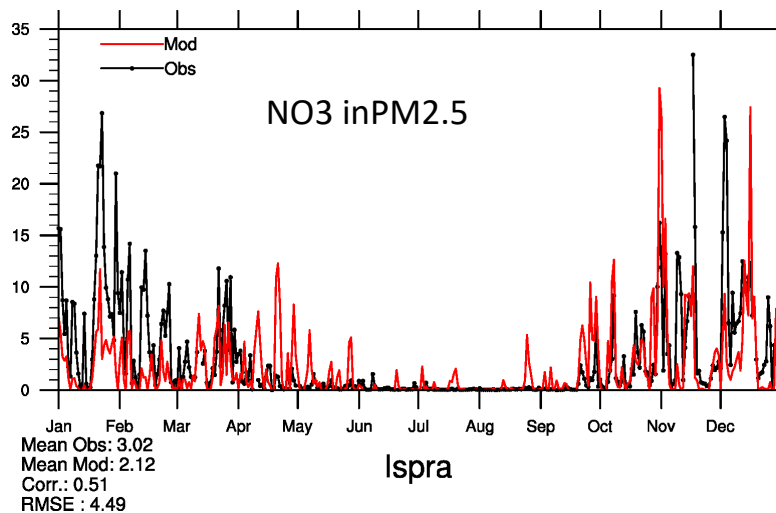
Testing EQSAM4clim for 2016



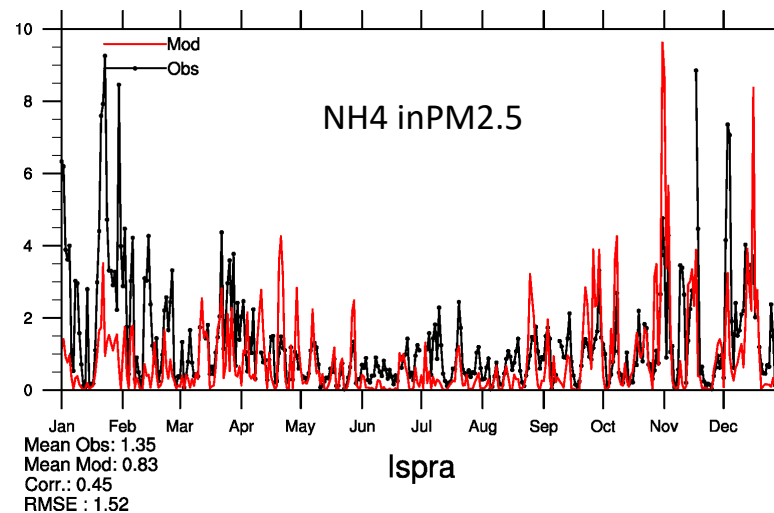
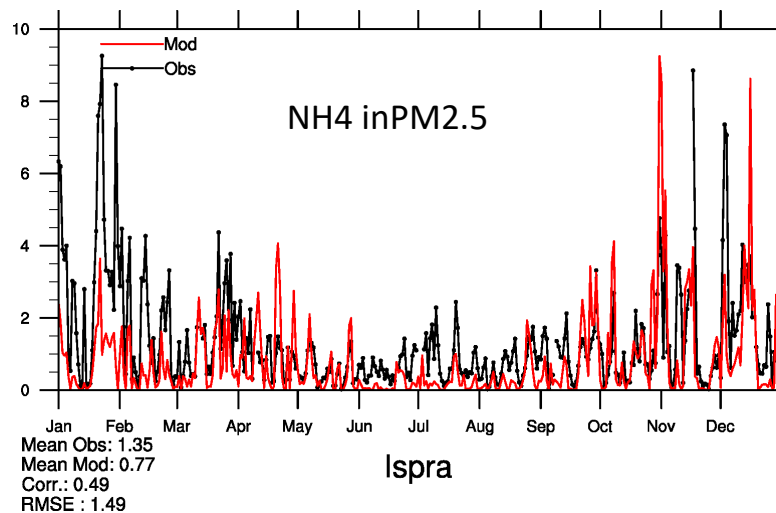
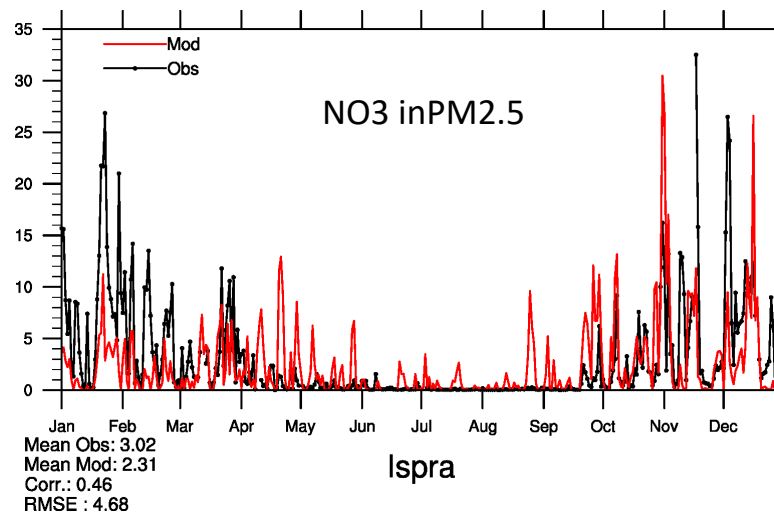
	NO3			NH4			HNO3	NH3	PM10	PM2.5
	Bias-y	R-y	IOA-yd	Bias-y	R-y	IOA-yd	Bias-y (%)			
MARS	9 %	0.82	0.89	-12 %	0.65	0.80	-22	66	-17	-14
Eq4clim	5 %	0.83	0.90	-14 %	0.64	0.79	-30	73	-24	-20
Rep18	13 %	0.83	0.90	-11 %	0.65	0.80	-31	68	-22	-18

y – yearly, d - daily

EQSAM4clim



MARS



NO_3^- in $\text{PM}_{2.5}$

	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 $\text{PM}_{2.5}$

EQSAM4clim: testing setups

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

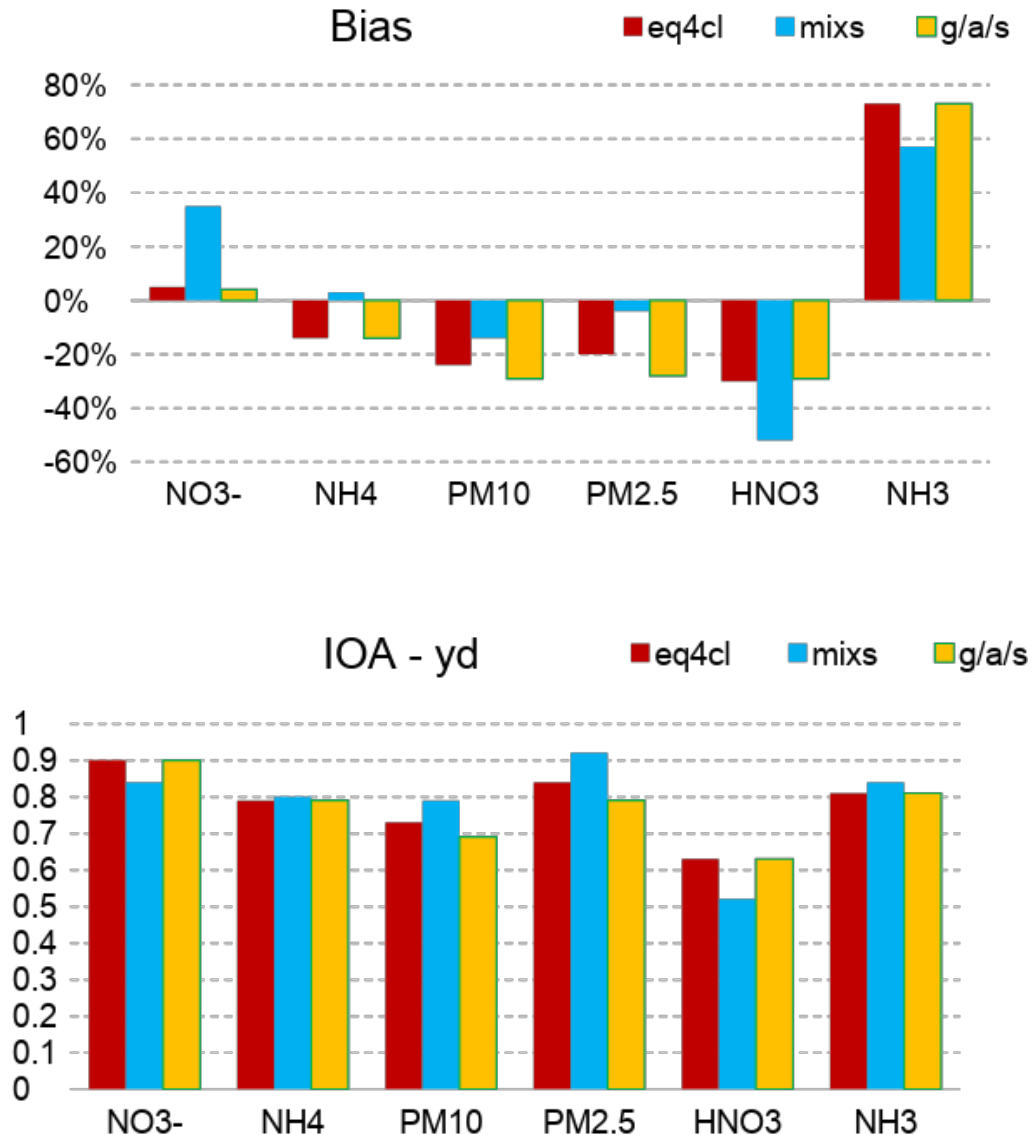
Ideally, all major cation/anions should be included for best result

Presently, base cations from mineral dust are not accounted for

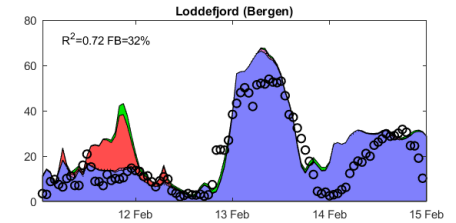
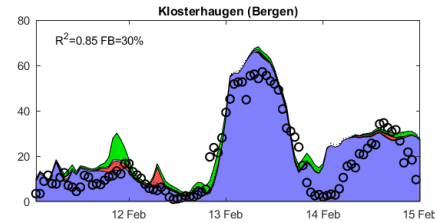
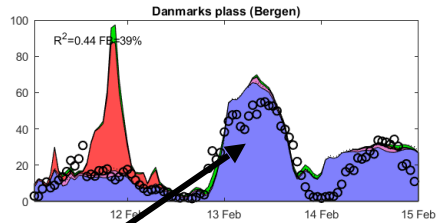
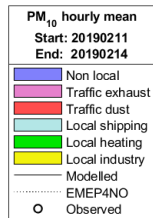
eq4cl – metastable aqueous aerosols, gas/aerosol partitioning (as in MARS)

mixs – equil. dissociation constant K_p for NH_4NO_3 not only $f(\text{RH}, T)$, but also $f(\text{composition})$: decreases with increasing $(\text{NH}_4)_2\text{SO}_4$ content

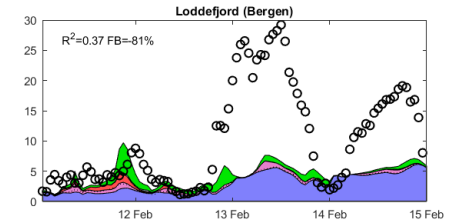
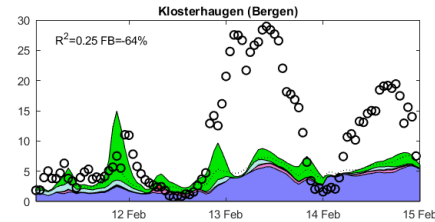
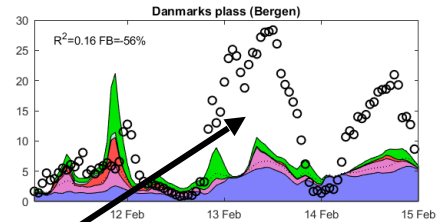
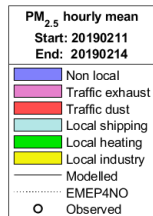
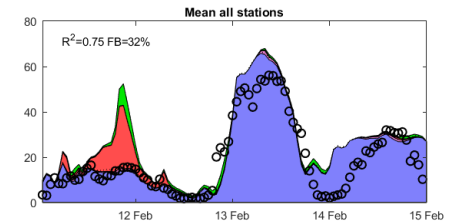
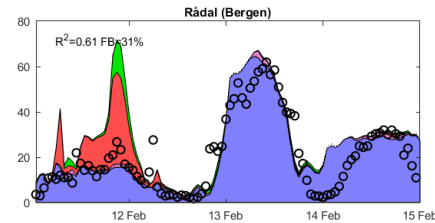
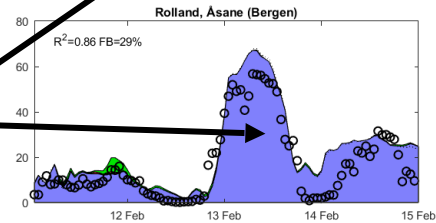
g/a/s – full gas/aerosol/solid equilibrium



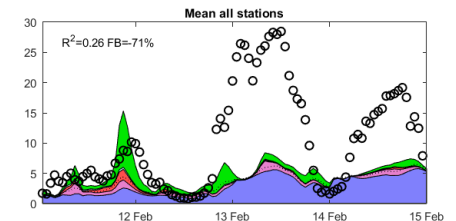
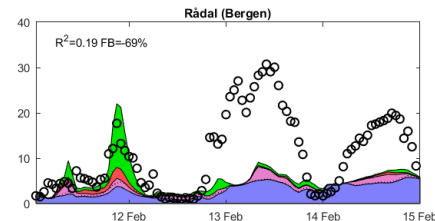
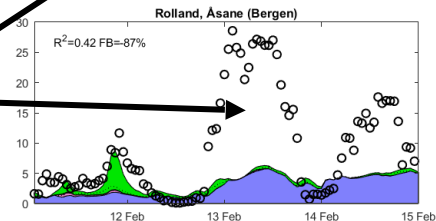
PM episode due to sea salt in Bergen (Norwegian west coast) 13.02.2019



Model
manages
PM10

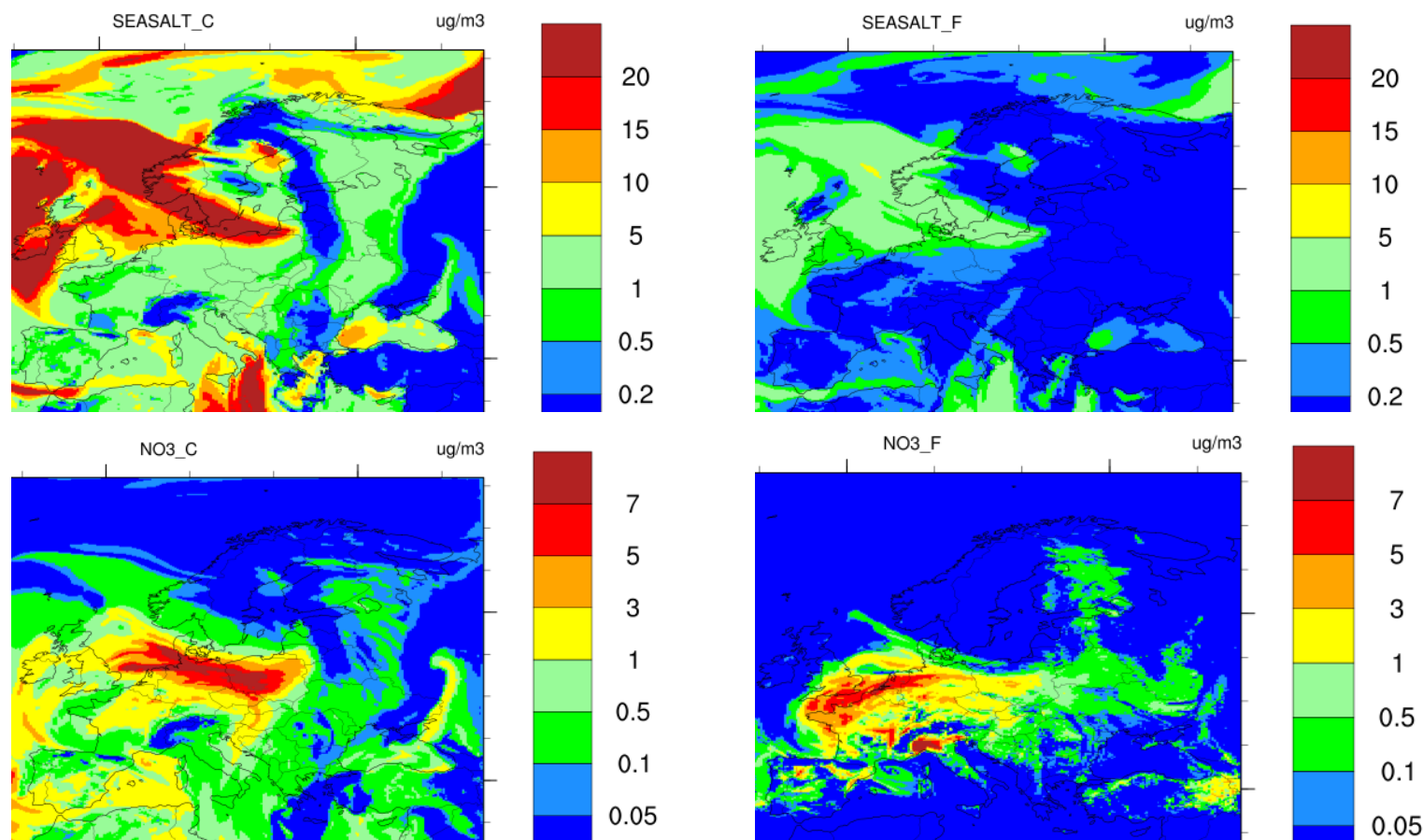


..but not
PM2.5



PM episode in Bergen (Norwegian west coast) 13.02.2019

air quality forecast using MARS



Coarse NO_3 (NaNO_3) formation,

but not NaNO_3 on fine sea salt

Also Na_2SO_4 is formed (actually preferential wrt $(\text{NH}_4)_2\text{SO}_4$)

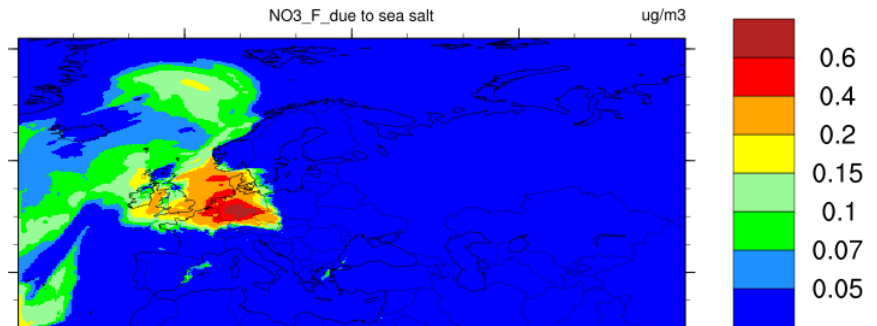
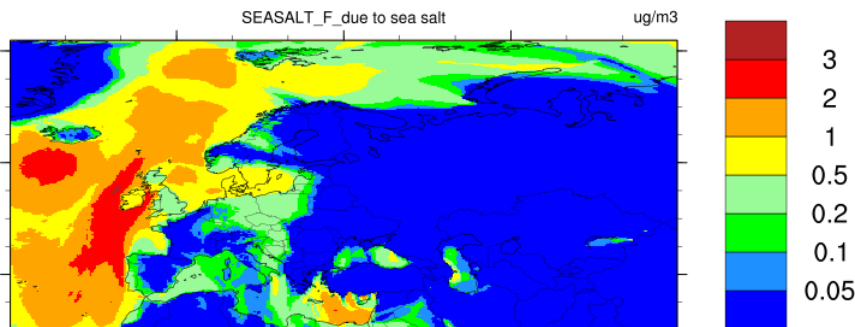
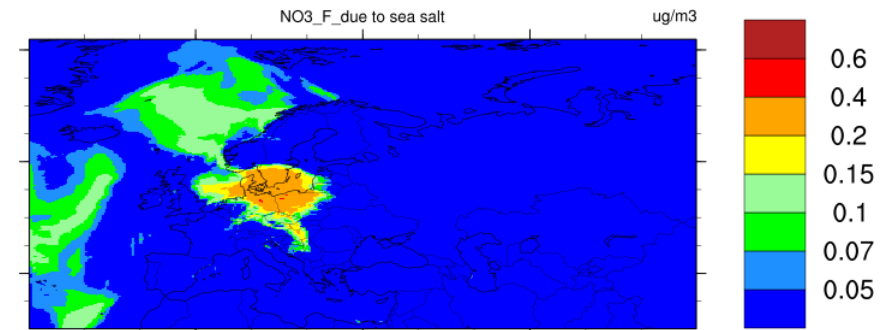
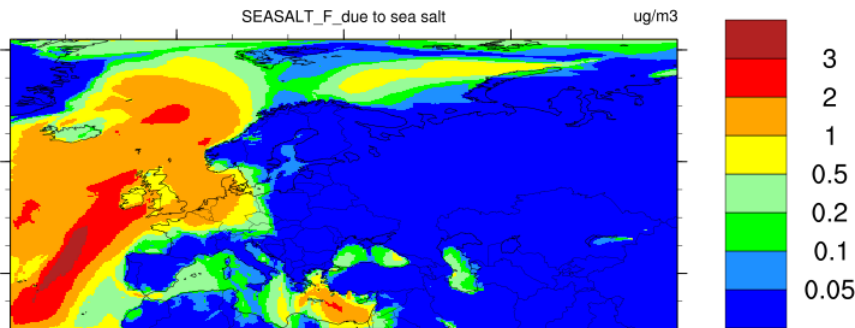
Could this (partly) explain the model failure????

EQSAM4clim

Formation of fine NO_3^+ due to fine sea salt

Sea salt

NO_3^+

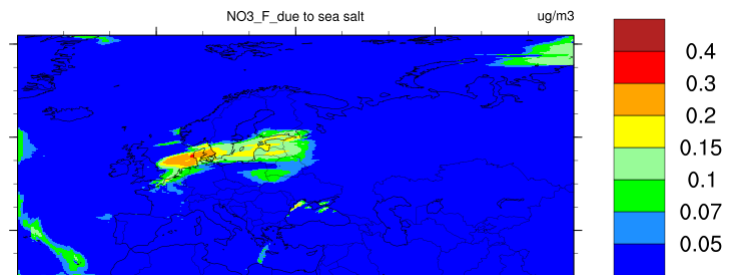
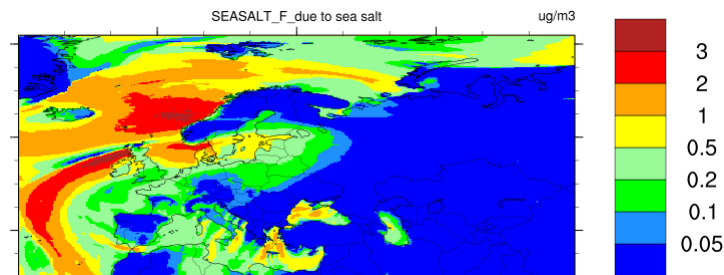
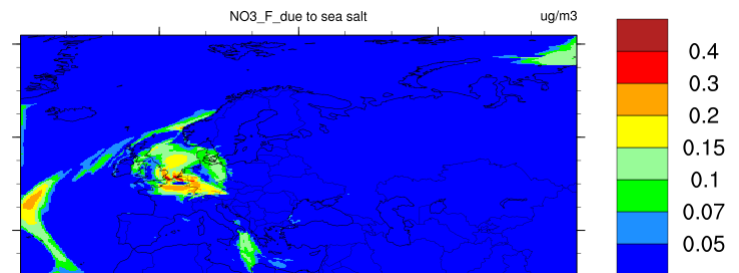
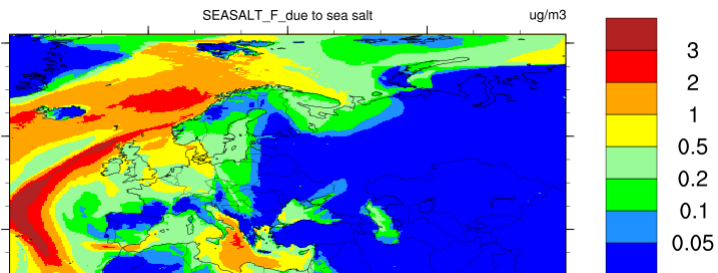
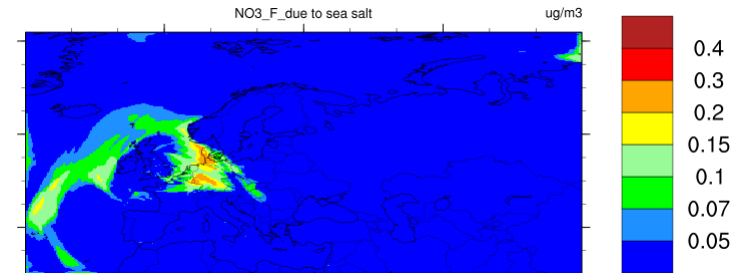
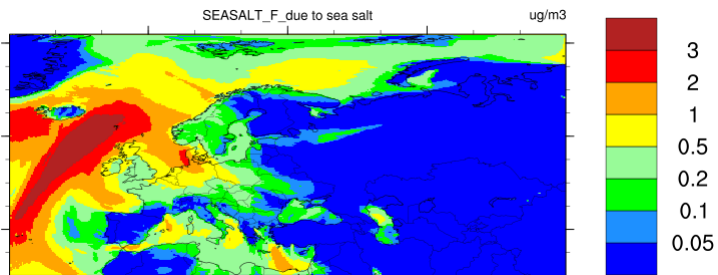


23-24 January 2016

Formation of fine NO_3^+ due to fine sea salt

Sea salt

NO_3^+

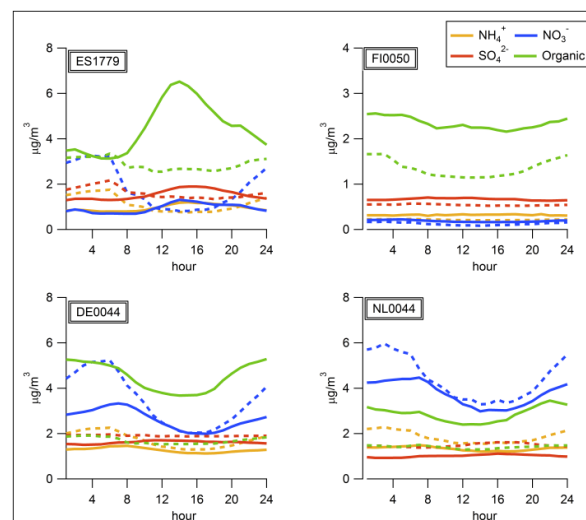
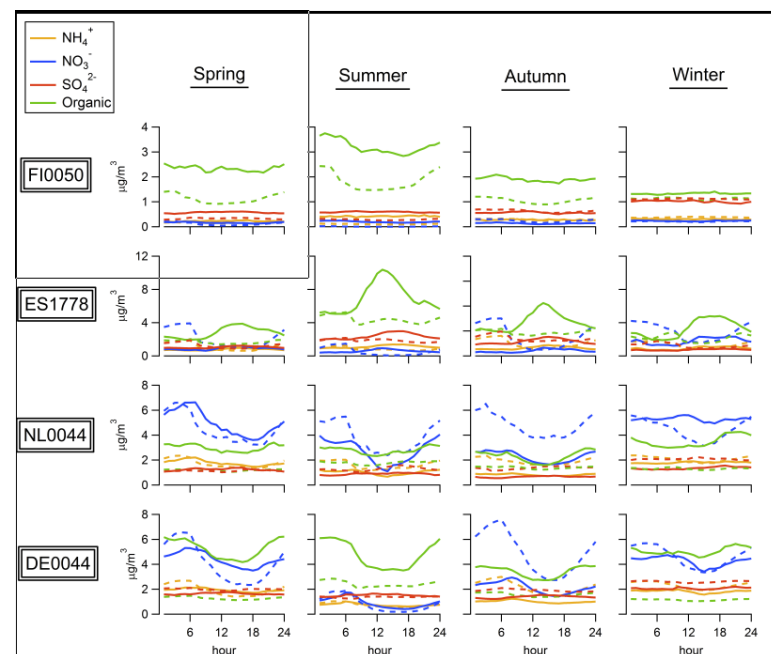
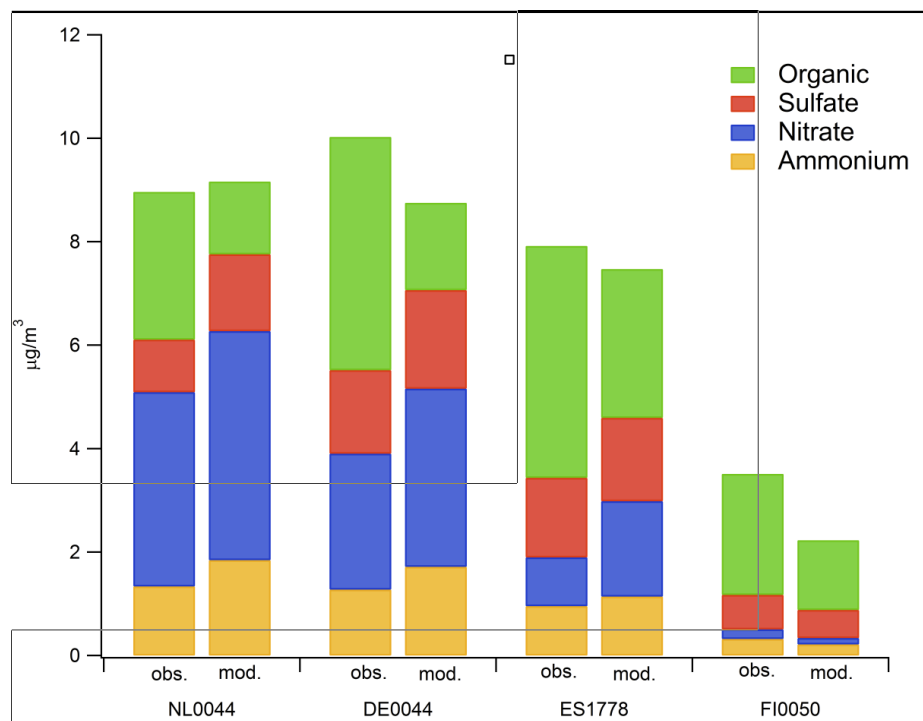


28-30 December 2016

Summary and outlook

- ★ The latest version of EQSAM - **EQSAM4clim** - has been implemented in the EMEP MSC-W model
- ★ Initial tests give positive results:
 - evaluation for 2016 - similar compared to MARS
 - inclusion of sea spray **NaCl in the equilibrium** allows formation of Na_2SO_4 and NaNO_3 (which can be important in coastal sea salt influenced regions)
 - several setups for equilibrium system complexity are tested - needs more study for diff regions (episodes!!), evaluation with observations (ACSM data, gas/aerosol)
 - more accurate calculation of **PM water** is expected, but depends on the setup (=completeness of cation/anion system)

Aerosol evaluation with ACSM (2012-2013)



EMEP Report 1/2017

Summary and outlook

- ★ EQSAM4clim will be one of the options to solve SIA in the Open Source (May 2019?) and after some testing next weeks will likely be used in model calculations for Report 2019

Further work

- ★ Extending to **base cations (Ca^{2+} , Mg^{2+} , K^{+})** from windblown and anthropogenic dust
- ★ Testing EQSAM4clim for coarse aerosols??

Many thanks go to Swen Metzger



for his assistance with EQSAM4clim implementation and consultancy regarding thermodynamics

Muchas gracias!