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The EMEP MSC-W model – history, status and future developments

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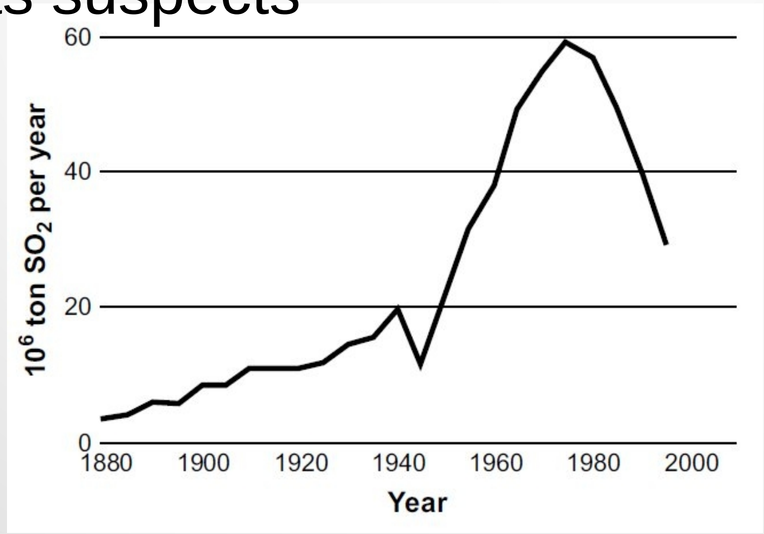
29/04/19

In the beginning: acid rain!

- Swedish/Norwegian scientists found major damage to fish stocks … suggested SO2 pollution from long-range transport was to blame….. with e.g. UK, Germany, Eastern Europe as suspects
  –

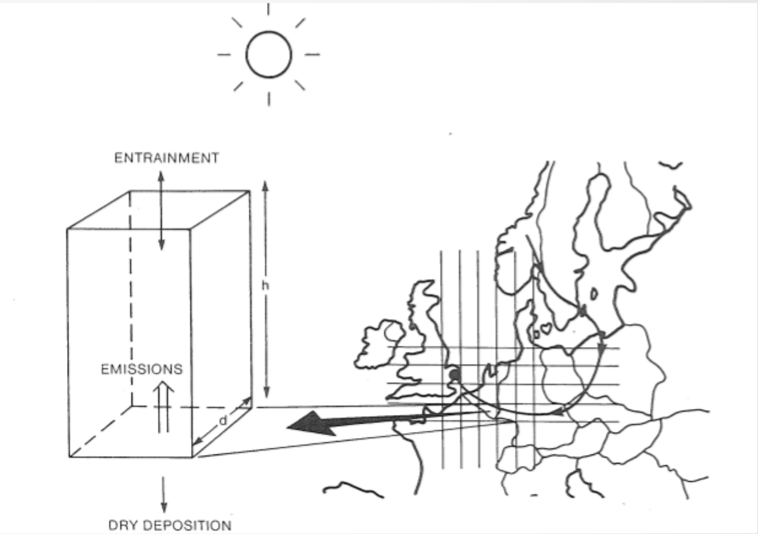


(Fenger 2009)

In the beginning: N=2 (Eliassen& Saltbones)

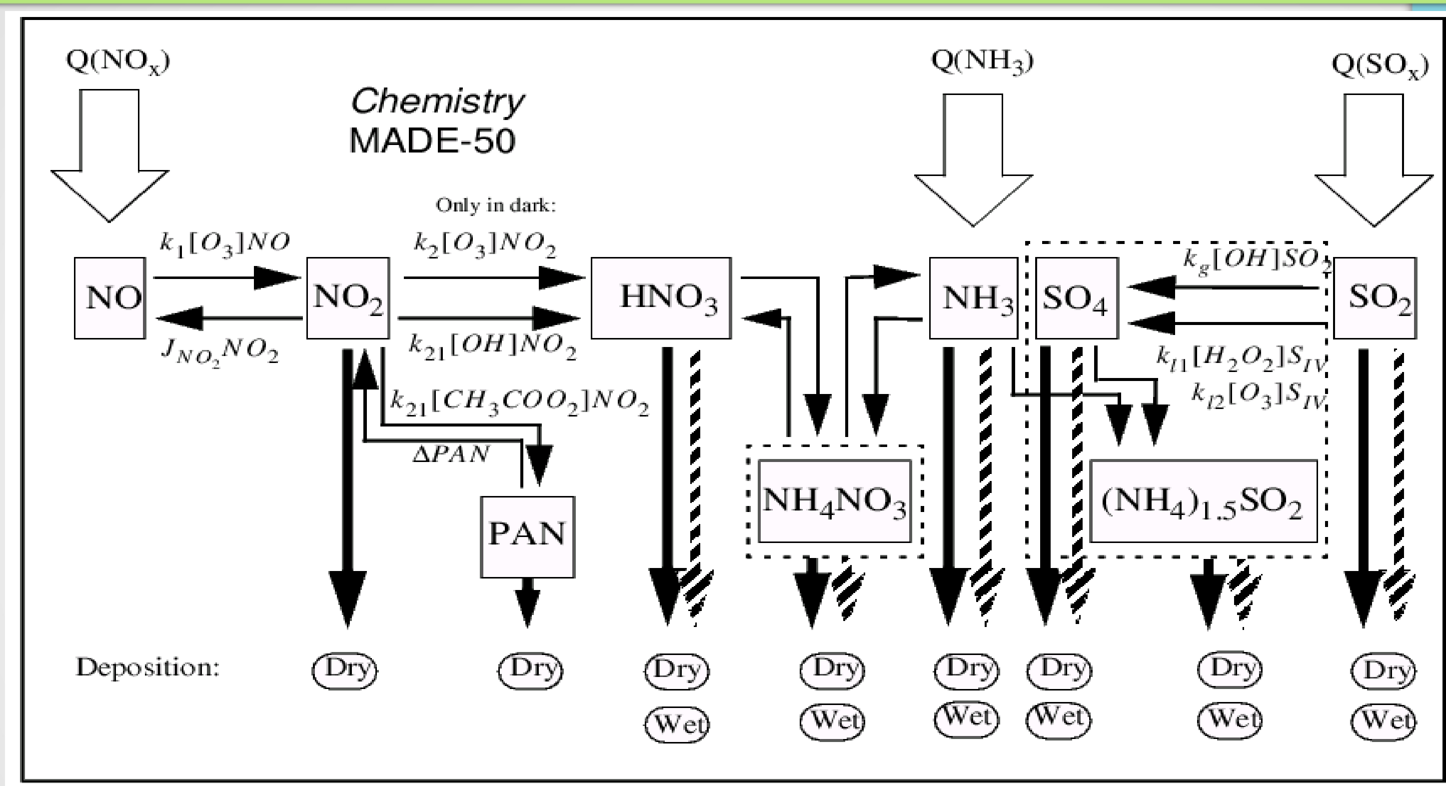
- OECD project (1970s)
  - Lagrangian model – enabled «fair» calculations of transport between countries
  - First long-range transport model
  - Used to calculate “blame” matrix
  - Sulphur

    => EMEP (MSC-E, MSC-W and CCE)
  -



Next step: NOx

N=5 Hov et al.



- NOx model, 1985 ...
  - Lagrangian, performed rather well. Basis of 1st Gothenburg multi-pollutant multi-effect Protocol

Onwards to Ozone (German forests...)

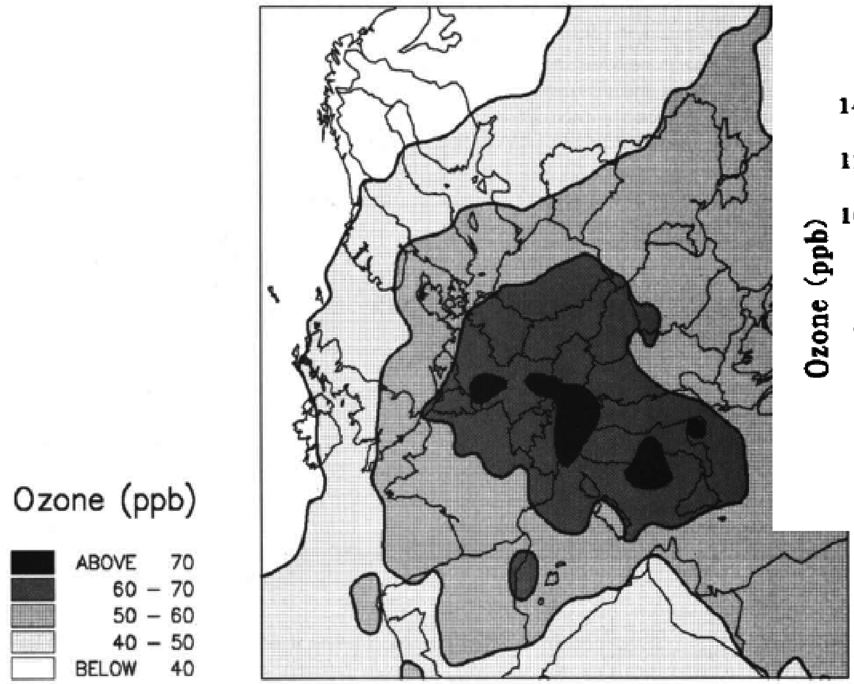
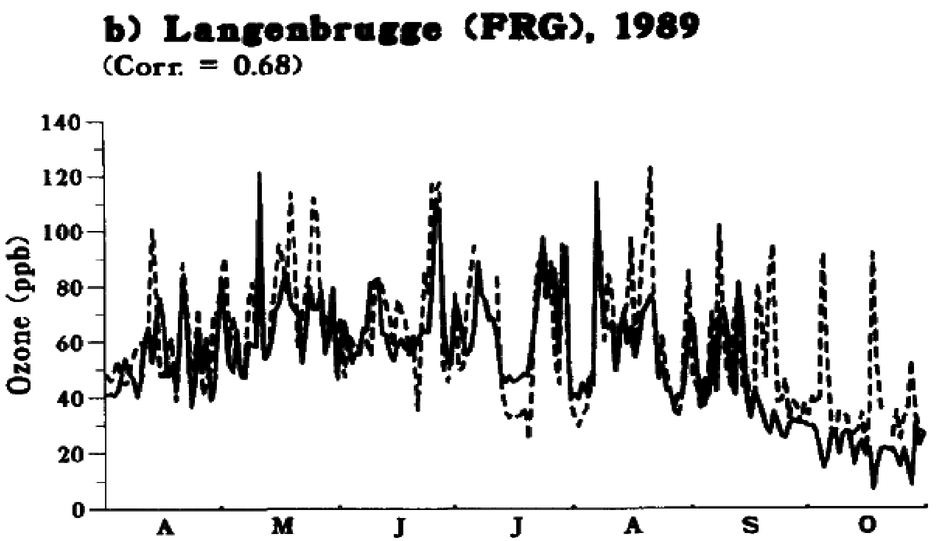


Fig. 8. Calculated mean of daily maximum ozone concentrations (ppb) July 1985.



- O3 model, Simpson, Atmos. Env., 1992, 1993 ...
  - Lagrangian- also performed rather well!

Eulerian: 1990s - today

N~7

- Eulerian acid deposition model
  - Erik Berge and Roar Skaalin
- Designed from scratch for parallel computing
  - Basis of today's fast code
  - EMEP models are almost perfectly scalable
- Eulerian acid deposition – mid 1990s (Berge et al.)
- Eulerian ozone – late 1990s (Jonson et al.)
- ‘Unified’ → Simpson et al, 2003

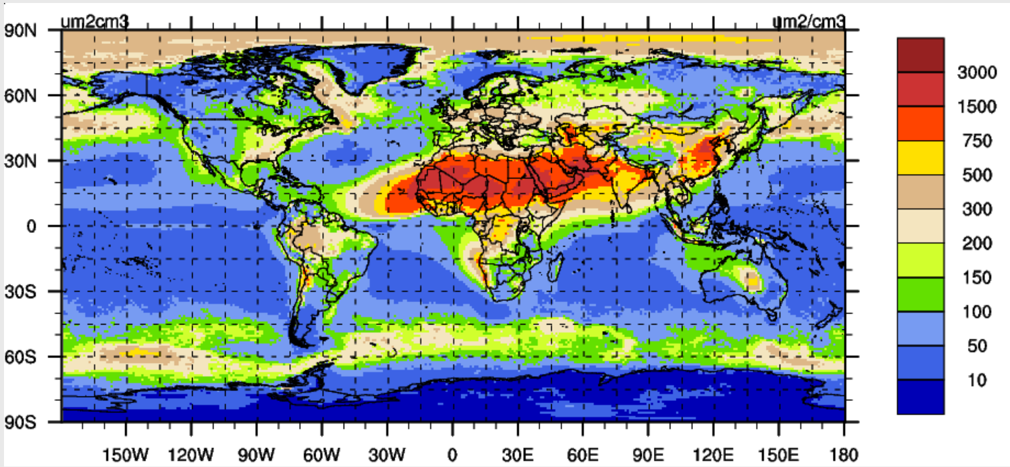
Public domain:

- First: 2007
- Why?
  - EMEP is funded by ~50 countries – should have an open model
  - To encourage use of EMEP model among Parties/scientists
  - To help improve model through co-operations
- To build a community!

Examples:

- EMEP4HR:
  - Application of EMEP model to Croatia
  - Focus on evaluation of turbulence and Hmix → new routines in core EMEP
- EMEP4UK
  - Application in UK, originally at 5km scale
  - Now down to 1km
  - Development of WRF+EMEP link
  - Extensive evaluation
  - Productive! (Vieno et al. papers)

EMEP model



- Chemical transport model
- Open source
- Ozone, Ndep, OA
- EMEP results underpin UN-ECE and EU emission control
- Large focus on comparison with observations, though mainly at European scale so far.
- Very flexible! (wrt scale, meteorology, chemistry)
- Very fast!
- Open source, with frequent updates
- Documentation: Simpson et al., Atmos. Chem. Physics, 2012, Annual EMEP reports

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Philosophy, concepts?

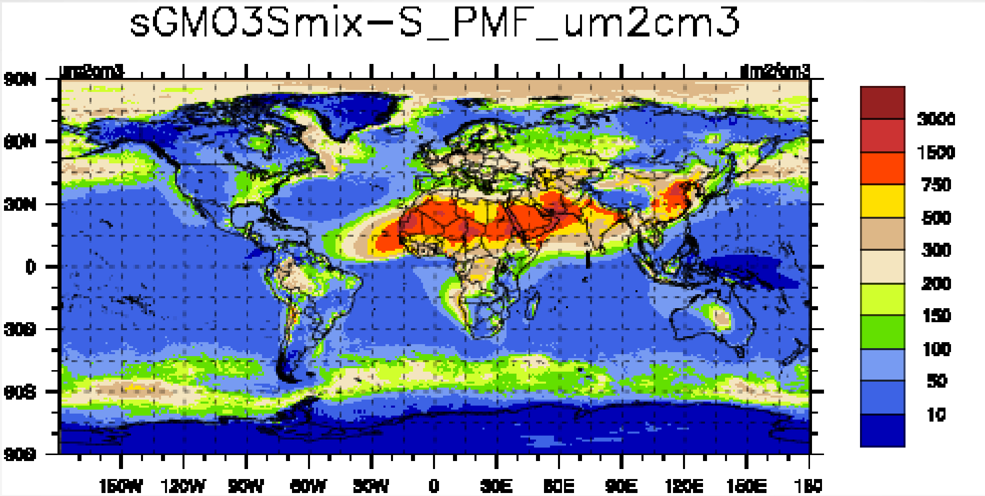
- Main ideas:
  - to capture the main atmospheric processes, keeping a balance between different components.
  - Make sure model is grounded in measurements!
  - … but, prefer sound science over best-possible result for specific compounds – try not to “tune”.
  - Make sure the model is useful!

Recent changes (since 2015 course)

- Aerosol surface area calculations
- Gas-particle reactions improved
- EmChem16x
- SHIPNOx
- Radiation (PAR calculations)
- Local Fraction (see Peter's talk)
- uEMEP link
- Even more flexible – emissions, meteorology

  - EMEP model: See Simpson et al., Atmos. Chem. Physics, 2012, Annual EMEP reports

Changes, e.g.: Aerosol surface area



- Aerosol surface area (S) now calculated using 'Gerber' functions
  - Empirical, we like ;-)
  - Avoids too much reliance on e.g. MARS/ISORROPIA/EQSAM
  - Unclear if high S due to fine-dust, sea-salt is correct
  - Large implications for e.g. modelling in Asia!
  - See Stadtler et al., ACP; 2018

Changes cont.: gas-aerosol interactions

- Gas-aerosol rates now depend on surface area
- Replaces older & cruder system
- Links inorganic chemistry to dust & sea-salt
- See Stadtler et al., ACP, 2018

$$k_X = \frac{1}{4} c_X \, S \, \gamma_X$$

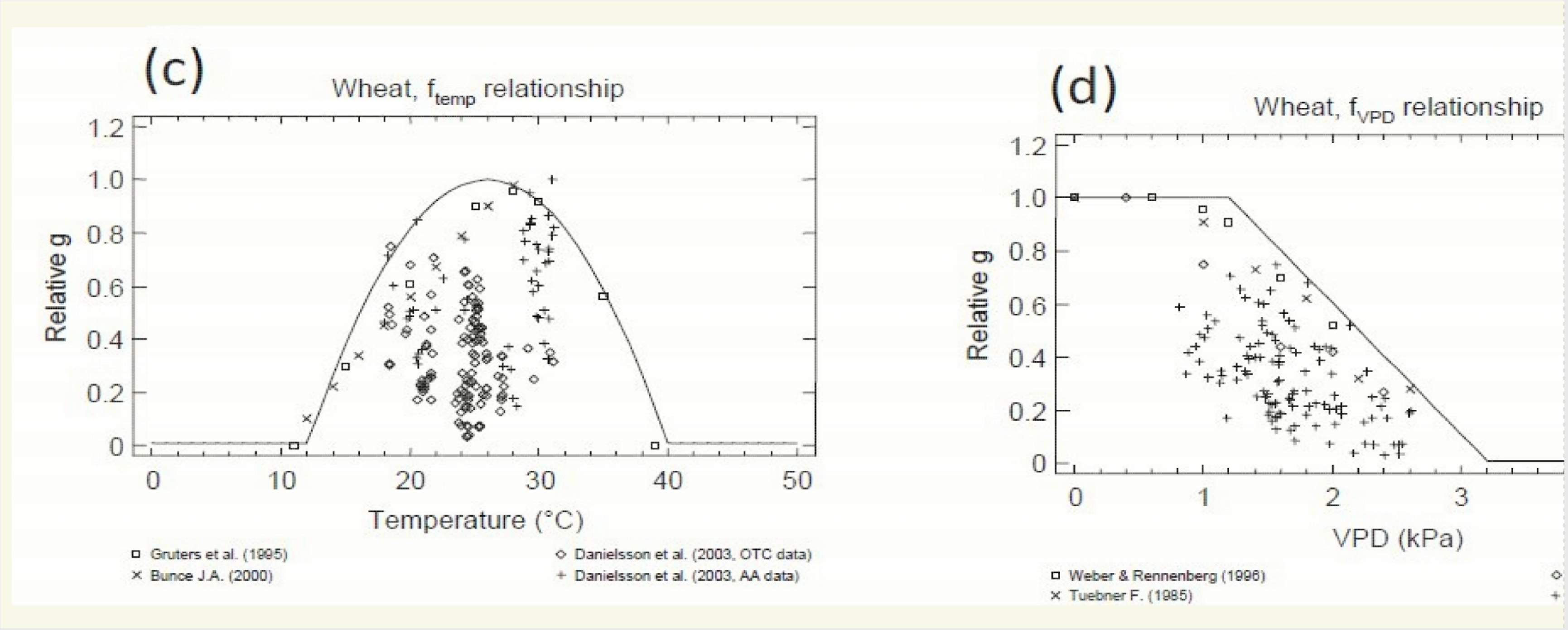
Table 1.1: Main aerosol-uptake reactions in rv4.7 EMEP model

Reaction		γ
$N_2O_{5\ (g)}$	$\longrightarrow 2\ HNO_{3\ (aq)}$	Options: Smix, SmixTen, or fixed values. See Sect.1.2.1
$HNO_{3\ (g)}$ + sea-salt$_c$	$\longrightarrow NO_{3,c}$	0.01
$HNO_{3\ (g)}$ + dust$_c$	$\longrightarrow NO_{3,c}$	0.02
$HO_{2\ (g)}$ + PM_c	$\longrightarrow \frac{1}{2} H_2O$	0.2
$O_{3\ (g)}$ + dust$_c$	$\longrightarrow HO_2$	1.0×10^{-6}

Notes: $NO_{3,c}$ represents coarse mode nitrate. These uptake reactions are applied whenever RH exceeds 40 %.

Changes – land-cover (Deposition methods unchanged: Jarvis-type stomatal conductance, DO3SE)

- Parameterises gsto as function of temperature, light, humidity, soil-moisture and phenology. .



EMEP/DO3SE – needs a lot of parameters!

Table S16: Land-cover specific parameters for stomatal conductance (DO_3SE) calculations

Code	g^m_{max}	f_{min}	f_{phen} factors								f_{light}	f_T			f_D		
			ϕ_a	ϕ_b	ϕ_c	ϕ_d	ϕ_e	ϕ_f	ϕ_{A_S}	ϕ_{A_E}	α	T_{min}	T_{opt}	T_{max}	D_{max}	D_{min}	$\Sigma D_{Crit.}$
	†						days	days	days	days		°C	°C	°C	kPa	kPa	kPa
CF	140	0.1	0.8	0.8	0.8	0.8	1	1	0	0	0.006	0	18	36	0.5	3	
DF	150	0.1	0	0	1	0	20	30	0	0	0.006	0	20	35	1	3.25	
NF	200	0.1	1	1	0.2	1	130	60	80	35	0.013	8	25	38	1	3.2	
BF	200	0.02	1	1	0.3	1	130	60	80	35	0.009	1	23	39	2.2	4	
TC	300	0.01	0.1	0.1	1	0.1	0	45	0	0	0.0105	12	26	40	1.2	3.2	8
MC	300	0.019	0.1	0.1	1	0.1	0	45	0	0	0.0048	0	25	51	1	2.5	
RC	360	0.02	0.2	0.2	1	0.2	20	45	0	0	0.0023	8	24	50	0.31	2.7	10
SNL	60	0.01	1	1	1	1	1	1	0	0	0.009	1	18	36	1.3	3	
GR	270	0.01	1	1	1	1	0	0	0	0	0.009	12	26	40	1.3	3	
MS	200	0.01	1	1	0.2	1	130	60	80	35	0.012	4	20	37	1.3	3.2	
IAM_CR	500	0.01	0.1	0.1	1	0.1	0	45	0	0	0.0105	12	26	40	1.2	3.2	8
IAM_DF	150	0.1	0	0	1	0	15	20	0	0	0.006	0	21	35	1	3.25	
IAM_MF	175	0.02	1	1	0.3	1	130	60	80	35	0.009	2	23	38	2.2	4	

Notes: † Units of g^m_{max} are mmole O_3 m^{-2} (PLA) s^{-1}

Simpson et al. ACP, 2012

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EMEP/DO3SE – and from 2017 a lot more --- added global landcover.. (but with very European surrogates)

Landcover	gmax	fmin	f_phen	#	#	#	#	#	Astart	Aend	flight	ftemp	#	#
LU	#	#	fac	fac	fac	fac	len	len	(rel-SGS)	(rel_EGS)	#	min	opt	max
NDLF_EVGN_TMPT_TREE	140	0.1	0.8	0.8	0.8	0.8	1	1	0	0	0.006	0	18	36
NDLF_EVGN_BORL_TREE	140	0.1	0.8	0.8	0.8	0.8	1	1	0	0	0.006	0	18	36
NDLF_DECD_BORL_TREE	150	0.1	0	0	1	0	20	30	0	0	0.006	0	20	35
BDLF_EVGN_TROP_TREE	150	0.1	0	0	1	0	20	30	0	0	0.006	0	20	35
BDLF_EVGN_TMPT_TREE	150	0.1	0	0	1	0	20	30	0	0	0.006	0	20	35
BDLF_DECD_TROP_TREE	150	0.1	0	0	1	0	20	30	0	0	0.006	0	20	35
BDLF_DECD_TMPT_TREE	150	0.1	0	0	1	0	20	30	0	0	0.006	0	20	35
BDLF_DECD_BORL_TREE	150	0.1	0	0	1	0	20	30	0	0	0.006	0	20	35
BDLF_EVGN_SHRB	60	0.01	1	1	1	1	1	1	0	0	0.009	1	18	36
BDLF_DECD_TMPT_SHRB	60	0.01	1	1	1	1	1	1	0	0	0.009	1	18	36
BDLF_DECD_BORL_SHRB	60	0.01	1	1	1	1	1	1	0	0	0.009	1	18	36
C3_ARCT_GRSS	270	0.01	1	1	1	1	0	0	0	0	0.009	12	26	40
C3_NARC_GRSS	270	0.01	1	1	1	1	0	0	0	0	0.009	12	26	40
C4_GRSS	270	0.01	1	1	1	1	0	0	0	0	0.009	12	26	40
CROP	270	0.01	1	1	1	1	0	0	0	0	0.009	12	26	40
BARE	-1	-1	-1	-1	-1	-1	0	-1	0	0	-1	-1	-1	-1

With LPJ-GUESS providing LAI, phenology for these non-European veg.

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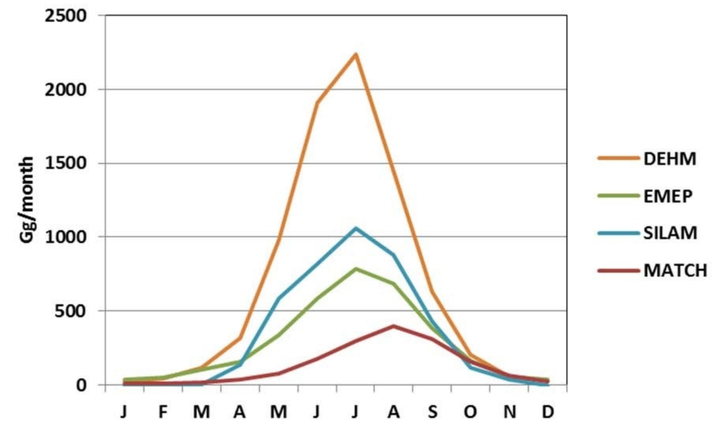
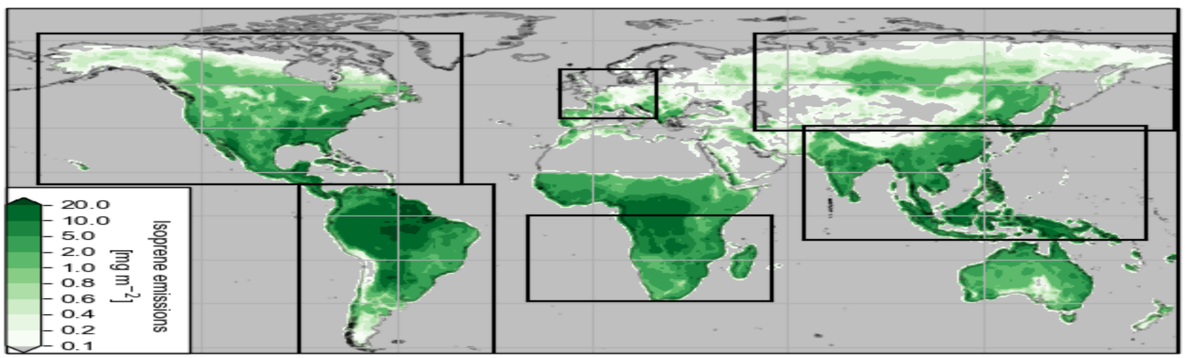
BVOC in EMEP – also changing

- All BVOC very uncertain (right)
- Global (below): mixes CLM & GLC2000 & EMEP emission factors (e.g. for TEMP_DEC_TREE).

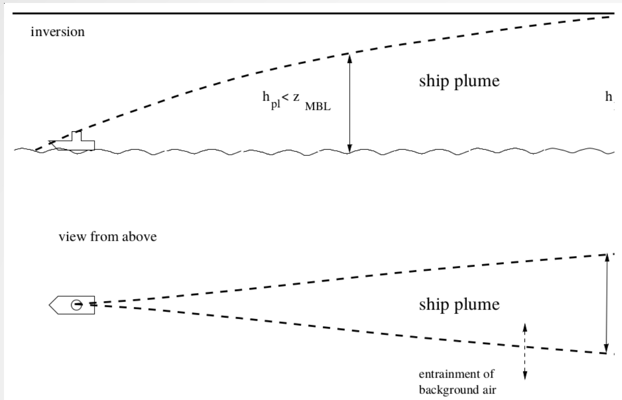


Langner et al., ACP, 2012



EMEP isoprene emissions (McFiggans et al., Nature, 2019)

Changes cont: ShipNOx



- Non-linearity of ozone chemistry can cause ship plumes to
  - Generate too much O3
  - Give too long lifetime for NOx

- ShipNOx:
- Pragmatic solution to provide faster conversion to HNO3 and reduce O3 production over oceans.
- Loosely (very!) based on GEOS-Chem PARANOX (Vinken et al, 2011)
- 50% of ship NO emitted as 'ShipNOx'

$$\begin{array}{llll} \mathrm{ShipNOx} + \mathrm{OH} & \Rightarrow & \mathrm{HNO_3} & \mathrm{R1} \\ \mathrm{ShipNOx} & \Rightarrow & \mathrm{HNO_3} & \mathrm{R2} \end{array}$$

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EMEP – coming soon....

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Coming soon...

- New chemical schemes:
  - EmChem19, CB6, CRI-emep
- BoxChem/GenChem
- EQSAM4
- ISOROPIA (restored)
- Updated land-cover (GLC2015-based)
- Bug-fix, radiation calculations (affects POD)
- Revised biogenic emissions (NO, DMS, ...) - via CAMS project
- Documentation!! (Update of 2012 ACP paper)

GenChem

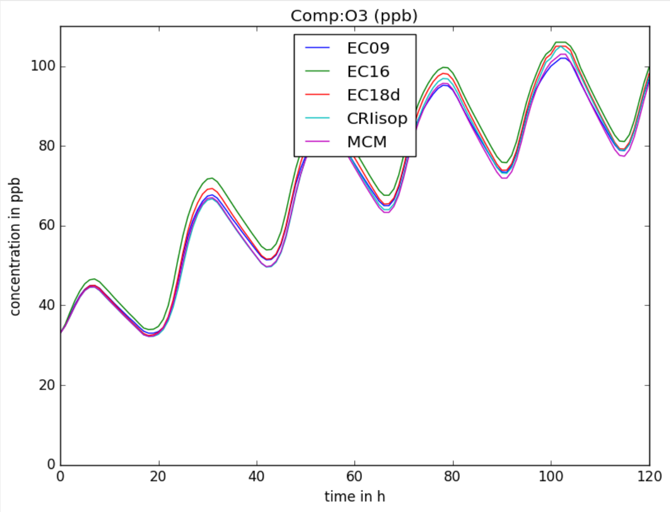
- A note on GenChem
- Pre-processor
  - Reads ascii chemical equations and description files
  - Produces all CM_ files
- 2013 statement: Needs code-clean and documentation before release. Will try to do in 2013…
- 2019 status: Oops! Actually, MCM changed, and all schemes had to re-calibrated. Code and documentation almost ready for release. Will try to do in 2019...

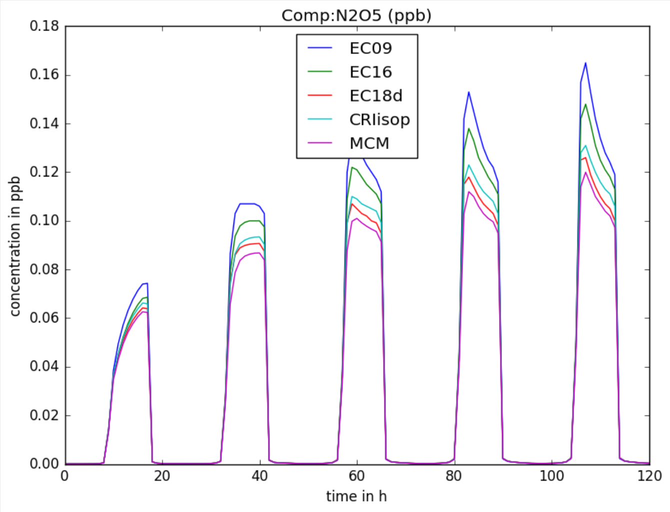
GenChem input

```
1.40e-12*exp(-1310*tinv)       NO + O3 = NO2 ;
KMT07                          OH + NO = HONO ;
3.60e-12*exp(270*tinv)         HO2 + NO = OH + NO2 ;
1.80e-11*exp(110*tinv)         NO + NO3 = 2.000 NO2 ;
1.40e-13*exp(-2470*tinv)       NO2 + O3 = NO3 ;
KMT08                          OH + NO2 = HNO3 ;
KMT09                          HO2 + NO2 = HO2NO2 ;
KMT10                          HO2NO2 = HO2 + NO2 ;
3.20e-13*exp(690*tinv)         OH + HO2NO2 = NO2 ;
4.50e-14*exp(-1260*tinv)       NO2 + NO3 = NO + NO2 ;
KMT03                          NO2 + NO3 = N2O5 ;
KMT04                          N2O5 = NO2 + NO3 ;
2.00e-11                       NO3 + OH = HO2 + NO2 ;
........
```

BoxChem/GenChem - Chemical mechanism toolbox

- BoxChem/GenChem ....
  - Updated EMEP mechanisms for comparability with latest MCM v3.3.1 (2017)
  - EmChem19, CRI, CB6
  - Evaluate new SOA schemes (Hodzic, JPC, 1.5D, ...)





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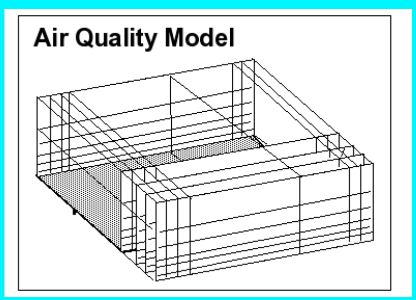
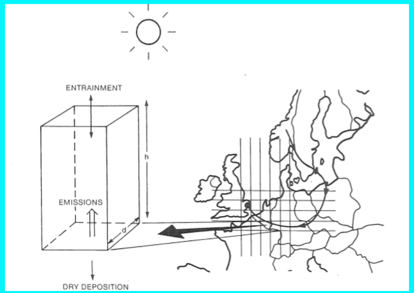
The EMEP/ESX/GenChem 'Family':

WRF - meteorology

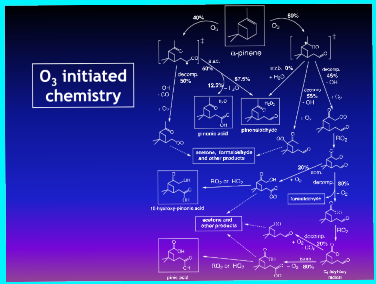
EMEP



ESX



BoxChem



GenChem - chemistry/aerosols

Almost final...

- The chemical schemes are getting more and more complex, e.g. SOA, aerosol schemes
- Difficult to summarise or address all issues related to EMEP model
- If interested in e.g. OA, or GenChem:
  - Please ask !

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Finally, some nice results ;-)

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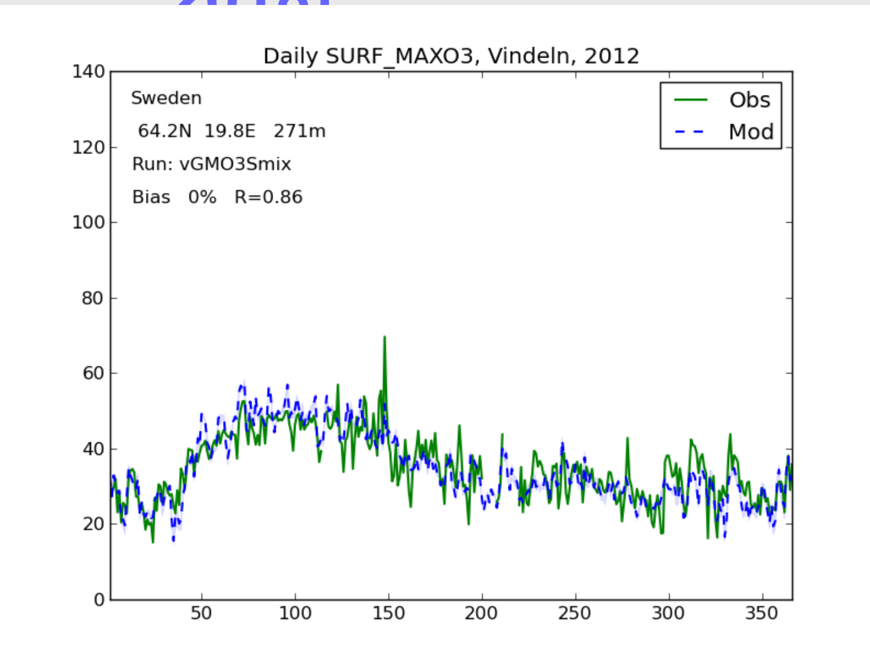
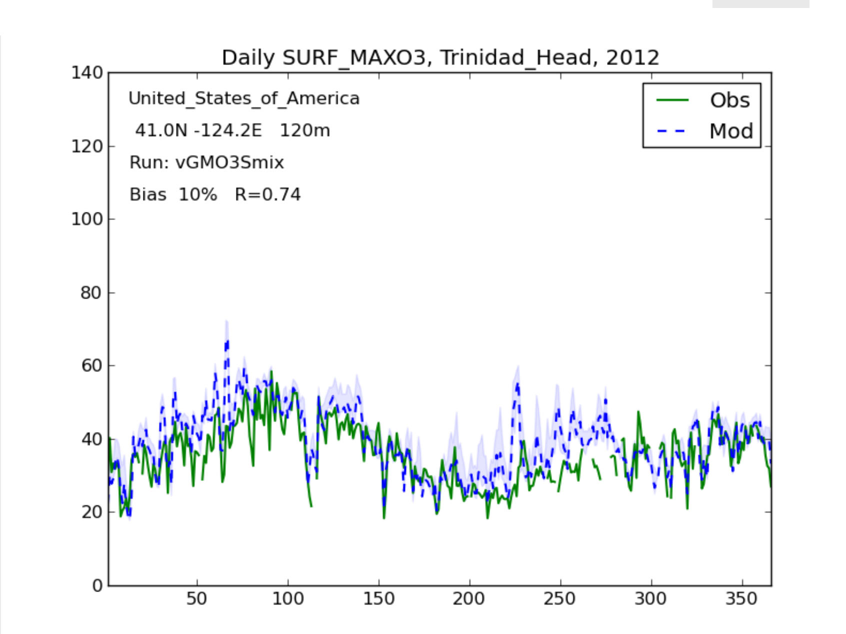
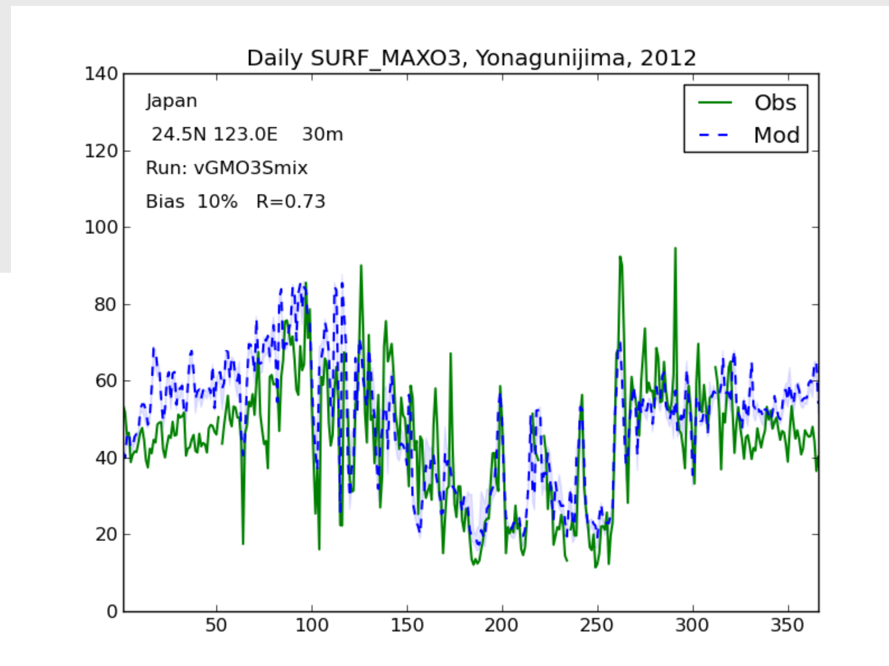
Can we model global ozone? (Mills et al., GCB, 2018)





- Daily max O3 (ppb) vs GAW data



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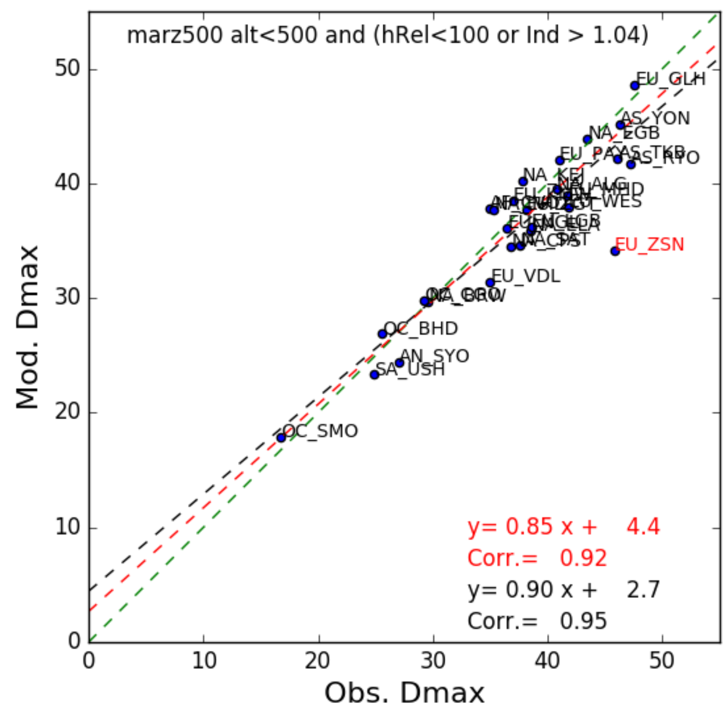
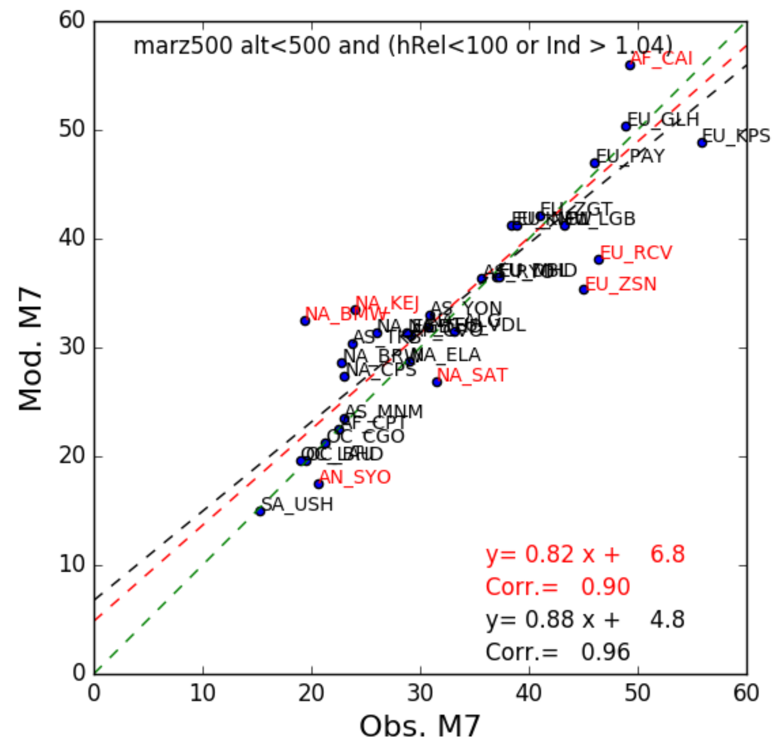
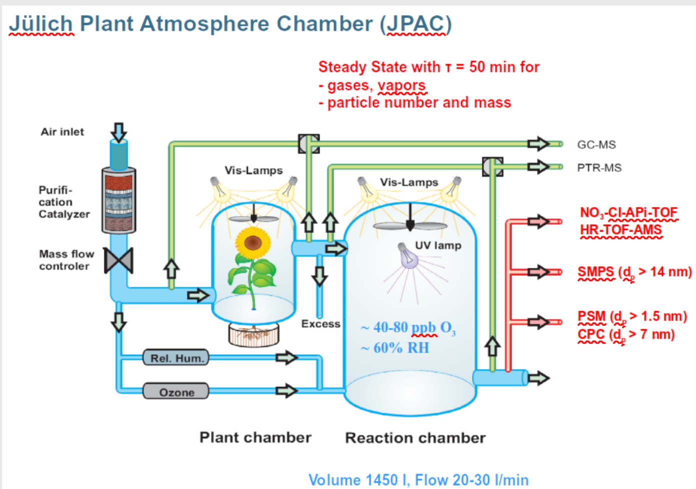
EMEP 3-D CTM performance – global (GAW)



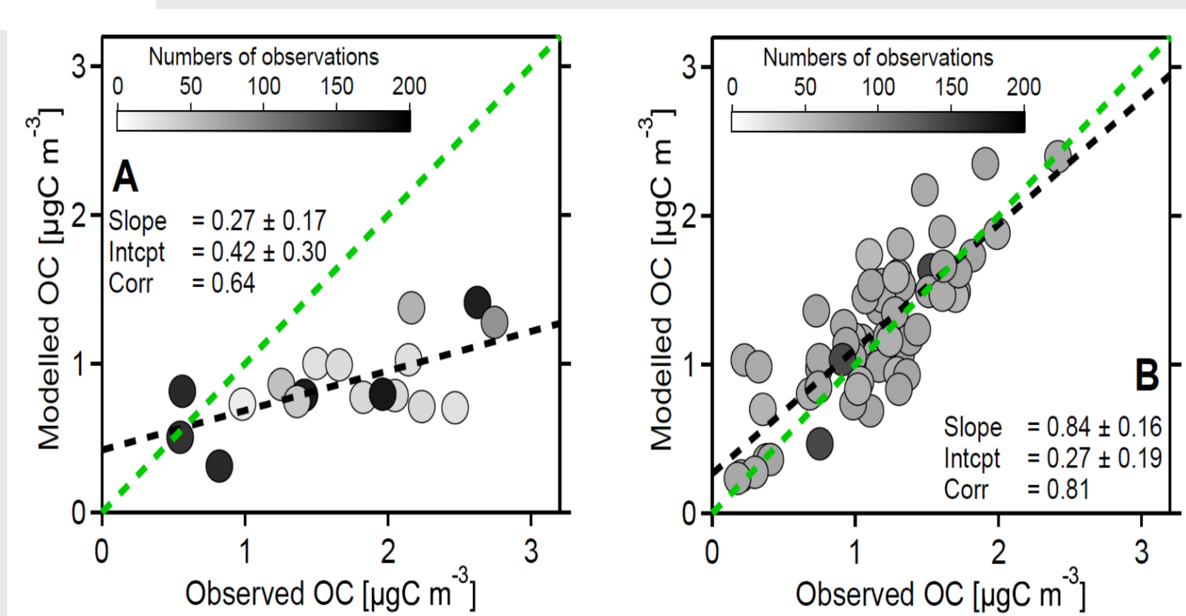
- Daily max O3, M7, 2012
- (From Mills et al 2018, SI)



Modelling organic aerosol – even simple schemes can work..... (McFiggans et al., Nature, 2018)



- BSOA modelled with fixed yields derived from JPAC chamber
- Compare with European (left) and America (right) OC



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Thanks for listening. The end!

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