Evaluating aerosol microphysics models: Observational datasets and plans for AEROCOM microphysics working group

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National Centre for Atmospheric Science
NATURAL ENVIRONMENT RESEARCH COUNCIL

AEROCOM microphysics working group

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At last year's AEROCOM workshop in Iceland, plan agreed for working group to evaluate aerosol microphysics models against range of available in-situ observations.

<u>Evaluate & document diversity of AEROCOM models in simulated number conc'n</u>

-- CN concentrations against CPC observations at GAW & other sites
-- CCN concentrations vs obs. from field campaigns & monitoring sites.
-- size distributions against DMPS observations at EUSAAR sites
-- size-resolved number concentrations & mean size against compilations of observed aerosol properties in literature (e.g. Heintzenberg et al, 2000, 2002).
-- vertical CN, CCN profiles from models against compilations of aircraft observations (e.g. TRACE-P, PEM-Tropics, INCA, UFA-EXPORT)

<u>***Please suggest other similar datasets that can be used to constrain models***</u>

<u>Experiments</u>:

-- Control simulation reference year 2006 (A2-CTRL-2006)
-- As CTRL but with condensation switched off (A2-SIZ1-2006)
-- As CTRL but with coagulation switched off (A2-SIZ2-2006)
-- As CTRL but with primary emissions of SO4 and BC/OC off (A2-SIZ3-2006)
-- As CTRL but with new particle formation switched off (A2-SIZ4-2006)

Use HCA-0 emissions in models to minimise differences between model simulations

Challenges when evaluating number concentrations

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Models characterise size distribution in many different ways
-- mass-only in aerosol types each with fixed size distribution (~10 aerosol tracers)
-- number & mass concentrations in size modes (20-30 aerosol tracers)
-- number & mass in concentrations size bins (100-200 aerosol tracers)

CCN observations retrieve CCN at many different supersaturations
(Not possible to make simple CCN diagnostics for models to output.)

CN measurements can use different minimum diameter (e.g. 3nm or 10nm).

Size distribution observations made across different size ranges.

Approach settled on at last workshop:
Instead of asking for extra complicated diagnostics, just make life simple:
Ask modelers to write "all-aerosol-tracer" output to AEROCOM database
And to provide README file with information on how size is handled in model.

Then can compare CN, CCN, size-resolved N ensuring consistent methodology.

Also ask modellers to interpolate to selected sites outputting at hourly resolution
-- makes separation into different air mass types possible
-- generate statistics of size distribution over daily cycle
-- how well do microphysics models reproduce new particle formation events?

Required output for aerosol microphysics group:

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-- Monthly-mean all-aerosol-tracer output on full 3D model grid (3D-M)
-- Daily-mean all-aerosol-tracer output over vertical profile at sites (1D-D)
-- Hourly-mean all-aerosol-tracer output at surface at sites (0D-H)
Use CMOR tables: Aerocom_table_1DD, Aerocom_table_0DH on website.

Selected sites:

GAW & ARM sites (CPC, nephelometer, aethalometer, some with lidar)
Alert, Barrow, Bondville, Mauna Loa, Neumayer, Samoa, South Pole, Southern Great Plains,

21 EUSAAR supersites (many with DMPS, AMS, lidar)
Aspreveten, Auchenworth, Birkenes, Cabauw, Finokalia, Harwell, Hohenpeissenberg, Hyytiala, Ispra, Jungfraujoch, Kosetice, K-puzta, Mace Head, Melpitz, Montseny, Moussala, Pallas, Preila, Puy de Dome, Valvihill, Zeppelin.

Additional sites with observations
Cape Grim, Cape Point, Capo San Juan, Elandsfontein, Guangzhou, Manaus, Monte Cimone, Mount Waliguan, Paverne, Shang Dianzi, Sonnblick, Summit, Tahkuse, Trinidad Head, Varrio

Need model README file giving full detail of size assumptions with model

Models intending to submit results:

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Following email questionnaire, many groups committed to submit results:

Model	Aerosol Dynamics	# of aerosol tracers	Contact
GLOMAP-bin	Bin-resolved (N,m)	~200	Dominick Spracklen (Leeds)
GLOMAP-mode	Modal (N,m)	30	Graham Mann (Leeds)
UKCA-UM	Modal (N,m)	30	Graham Mann (Leeds)
ECHAM-HAM	Modal (N,m)	25	Kai Zhang (MPI-Hamburg)
ECHAM-HAMMOZ	Modal (N,m)	25	Kai Zhang (MPI-Hamburg)
GISS-MATRIX	Moments (N,m)	60	Susanne Bauer (GISS)
EMAC [ECHAM-MESSy]	Modal (N,m)	30+	Kirsty Pringle (MPI-Mainz)
NCAR CAM4-MAM	Modal (N,m)	31/15	Xiaohong Liu (PNNL)
TM5	Modal (N,m)	25	Elisabetta Vignati (JRC)
CCCma AGCM4	PLA-bin (N,m)	240	Knut Van Salzen (Env Canada)
GISS-TOMAS	Bin (N,m)	~100?	Yunha Lee (Carnegie Mellon)
Nor-AGCM	Modal (N,m)	~20?	Trond Iversen (Norway Met.)
GEOS5-GOCART	Mode & bin (m-only)	~20	Peter Colarco (NASA GSFC)
ECHAM-HAM* &-SALSA	Mode (N,m), Bin (N,m)	~25, ~70	Risto Makkanen (Univ Helsinki)

Global Model of Aerosol Processes (GLOMAP)

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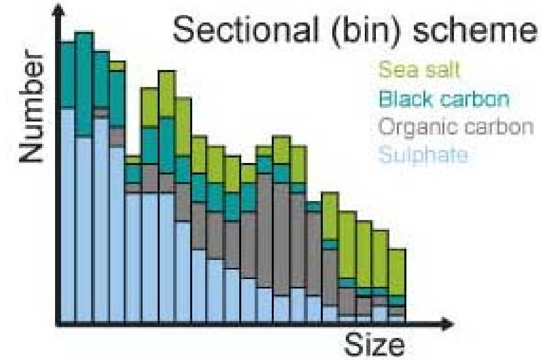

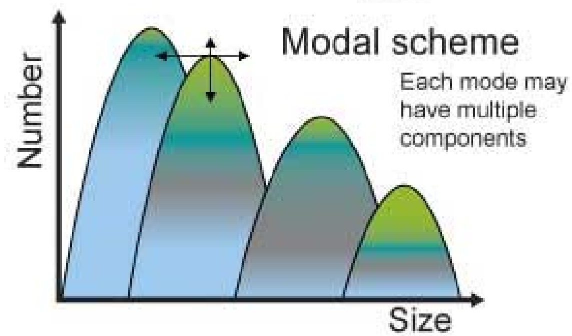

Global CTM forced by 6-hourly ECMWF winds

Usually run at T42L31 (2.8ºx2.8º) resolution

Sectional aerosol scheme: 20 bins, 3 nm – 20 μm
Modal scheme: 7 or 4 log-normal modes

Chemistry usually driven by offline oxidants,
now coupled to CTM chemistry

Aerosol transport, new particle formation, growth
by coagulation, condensation, cloud processing.

Wet and dry deposition of gases & aerosol particles

Emissions of DMS → SO_2 → H_2SO_4; monoterpenes → biogenic SOA

Primary emissions of sea salt, dust,
black & organic carbon (fossil and biofuels, vegetation fires)

Nucleation via binary homogeneous nucleation of H_2SO4-H_2O
and also now implemented boundary layer nucleation mechanism

GLOMAP-bin : Spracklen et al. (2005), Spracklen et al (2008)
GLOMAP-mode: Manktelow et al (2007), Mann et al (in prep, 2009).

Example model README file for GLOMAP-mode:

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```
The following describes the all-aerosol-tracer information for GLOMAP-mode.
Contact: Graham Mann (University of Leeds, U.K.) gmann@env.leeds.ac.uk

Model setup for AEROCOM simulations uses 7 log-normal modes
Mode 1 is   soluble nucleation   with cpts SO4,POM
Mode 2 is   soluble Aitken       with cpts SO4,BC,POM
Mode 3 is   soluble accumulation with cpts SO4,BC,POM,NaCl,dust
Mode 4 is   soluble coarse       with cpts SO4,BC,POM,NaCl,dust
Mode 5 is insoluble Aitken       with cpts BC,POM
Mode 6 is insoluble accumulation with cpts dust
Mode 7 is insoluble coarse       with cpts dust

Aerosol tracers then are  19 mmrtrnn  values for components    (nnn=01 to 19)
                           4 mmrtrnn  values for water-content (nnn=20 to 23)
                           7 conccnxx values for number concns (xx =01 to 07)

Aerosol tracer ordering in CMOR-compliant netCDF files are:
mmrtr01       --- SO4  mmr in soluble   nucleation   mode
mmrtr02       --- POM  mmr in soluble   nucleation   mode
mmrtr03       --- SO4  mmr in soluble   Aitken       mode
mmrtr04       --- BC   mmr in soluble   Aitken       mode
mmrtr05       --- POM  mmr in soluble   Aitken       mode
mmrtr06       --- SO4  mmr in soluble   accumulation mode
mmrtr07       --- BC   mmr in soluble   accumulation mode
mmrtr08       --- POM  mmr in soluble   accumulation mode
mmrtr09       --- NaCl mmr in soluble   accumulation mode
mmrtr10       --- dust mmr in soluble   accumulation mode
mmrtr11       --- SO4  mmr in soluble   coarse       mode
mmrtr12       --- BC   mmr in soluble   coarse       mode
mmrtr13       --- POM  mmr in soluble   coarse       mode
mmrtr14       --- NaCl mmr in soluble   coarse       mode
mmrtr15       --- dust mmr in soluble   coarse       mode
mmrtr16       --- BC   mmr in insoluble Aitken       mode
mmrtr17       --- POM  mmr in insoluble Aitken       mode
mmrtr18       --- dust mmr in insoluble accumulation mode
mmrtr19       --- dust mmr in insoluble coarse       mode
mmrtr20       --- H2O  mmr in soluble   nucleation   mode
mmrtr21       --- H2O  mmr in soluble   Aitken       mode
mmrtr22       --- H2O  mmr in soluble   accumulation mode
mmrtr23       --- H2O  mmr in soluble   coarse       mode
```

Example model README file for GLOMAP-mode:

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```
conccnmode01  --- no. conc in soluble   nucleation   mode
conccnmode02  --- no. conc in soluble   Aitken       mode
conccnmode03  --- no. conc in soluble   accumulation mode
conccnmode04  --- no. conc in soluble   coarse       mode
conccnmode05  --- no. conc in insoluble Aitken       mode
conccnmode06  --- no. conc in insoluble accumulation mode
conccnmode07  --- no. conc in insoluble coarse       mode

Molar masses (mm) and densities (rho) of the aerosol components used for the mmr are:
SO4  : mm=0.098   kg/mol, rho=1769 kg/m3
BC   : mm=0.012   kg/mol, rho=1500 kg/m3
POM  : mm=0.0168  kg/mol, rho=1500 kg/m3
NaCl : mm=0.05844 kg/mol, rho=1600 kg/m3
dust : mm=0.100   kg/mol, rho=2650 kg/m3

H2O  : mm=0.018   kg/mol, rho=1000 kg/m3

Geometric standard deviations (sigma) for the 7 modes are constant as:
sigma (soluble   nucleation  ) = 1.59
sigma (soluble   Aitken      ) = 1.59
sigma (soluble   accumulation) = 1.59
sigma (soluble   coarse      ) = 2.00
sigma (insoluble Aitken      ) = 1.59
sigma (insoluble accumulation) = 1.59
sigma (insoluble coarse      ) = 2.00

Geometric mean diameter (Dpi) for mode i is calculated as:
Dpi^3=6.0*dvoli/pi/explogsqsigmai

where explogsqsigmai=exp(4.5*alog(sigmai)*alog(sigmai))
and   dvoli=sumj(mdij*mmj/(avc*rhoj))
and   mdij=mmrtrnn*(mm_da/mm)*(aird/conccni)

(nn is the index of the tracer mmr for mode i component j).
(conccni is the number concentration in mode i)
```

Influence of microphysics on CN, CCN, AOD, mass

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In addition to scoring vs observations, evaluate diversity in simulated influence of primaries/nucleation/coagulation/condensation on simulated CN, CCN, mass, AOD

Table 2. Summary of ground level contribution from primary particles (PR), boundary layer nucleation (BLN) and upper tropospheric nucleation (UTN) to ground level total number (CN) and cloud condensation nuclei (CCN) concentrations at 0.2% and 1.0% supersaturations. The marine regions refer to west of North America (NAM), west of South America (SAM), west of North Africa (NAF), west of South Africa (SAF), and East of North-East Asia (NEA) (see Figure 7).

	CN		CCN(1.0%)		CCN(0.2%)	
Region	Tot [cm^{-3}]	PR-UTN-BLN [%]	Tot [cm^{-3}]	PR-UTN-BLN [%]	Tot [cm^{-3}]	PR-UTN-BLN [%]
Total Global	1064	27-25-47	513	49-33-18	314	61-31-8
Total Marine	758	19-33-48	331	41-44-15	204	52-40-9
NAM	596	20-63-18	384	28-63-8	396	36-56-9
SAM	567	14-41-45	273	31-58-11	148	41-53-7
NAF	1003	12-31-57	413	28-52-20	414	36-48-15
SAF	619	23-41-36	345	40-50-10	266	48-45-7
NEA	1423	35-35-30	877	52-35-13	886	62-30-8
Total Continental	1921	36-18-46	1024	57-23-20	625	69-23-7
Europe	2611	47-11-42	1647	63-15-22	932	67-24-10
Africa	1279	50-20-29	900	63-25-12	719	71-24-6
N. America	2600	20-12-69	1079	40-24-36	554	51-32-17
S. America	1713	36-15-49	922	61-25-14	613	71-26-3
N. Asia	1119	22-26-53	554	38-34-28	288	56-31-13
SE Asia	4543	46-14-40	2443	70-15-14	1384	83-13-4
Oceania	1335	21-20-59	778	34-31-36	431	51-38-11

Merikanto et al (2009)

CN concentrations (GLOMAP-mode)

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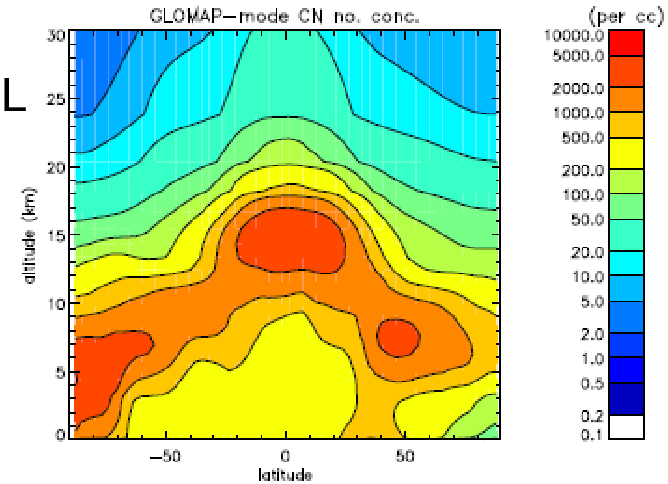
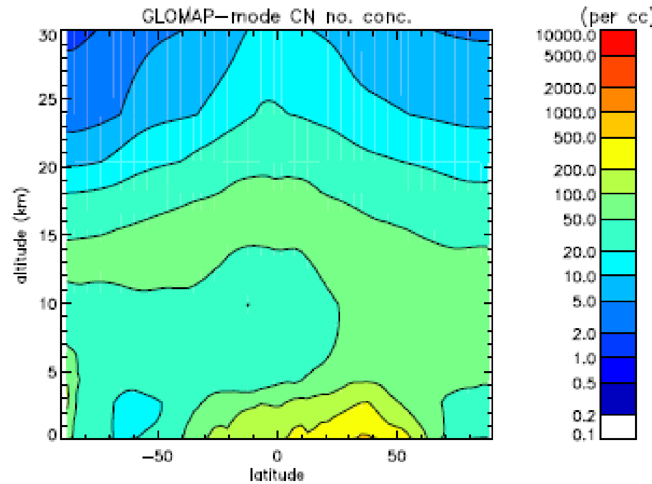
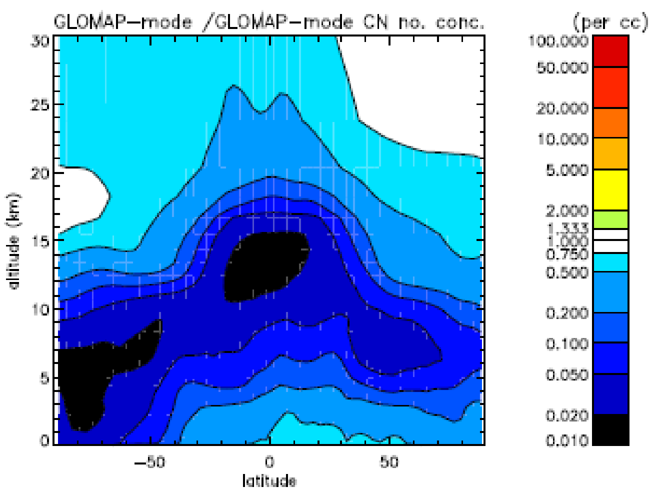
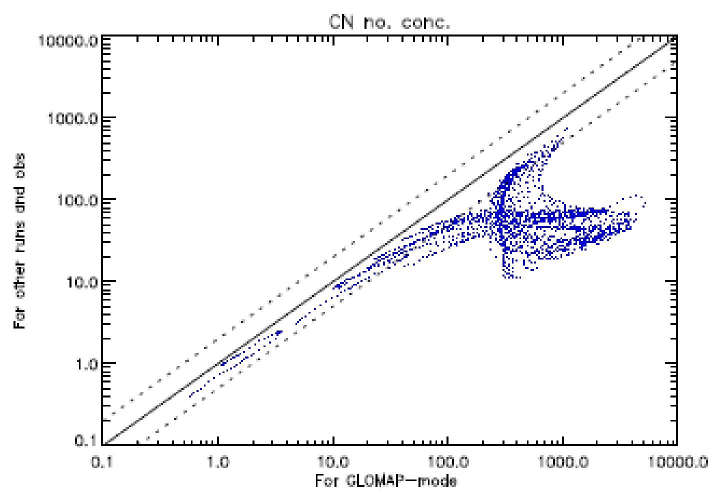
A2-CTRL
2006





A2-SIZ4
2006
(nucleation switched off)





Switching nucleation off removes observed CN peak in Upper Troposphere

CN concentrations (GLOMAP-mode)

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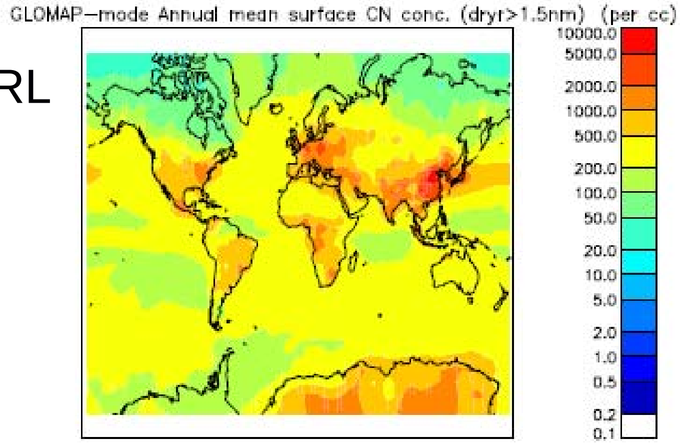
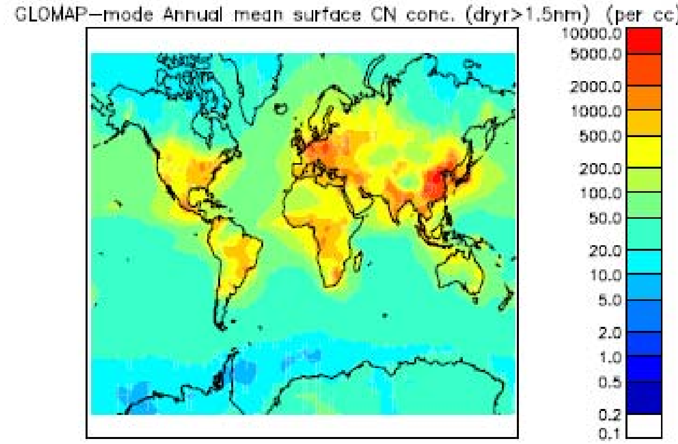
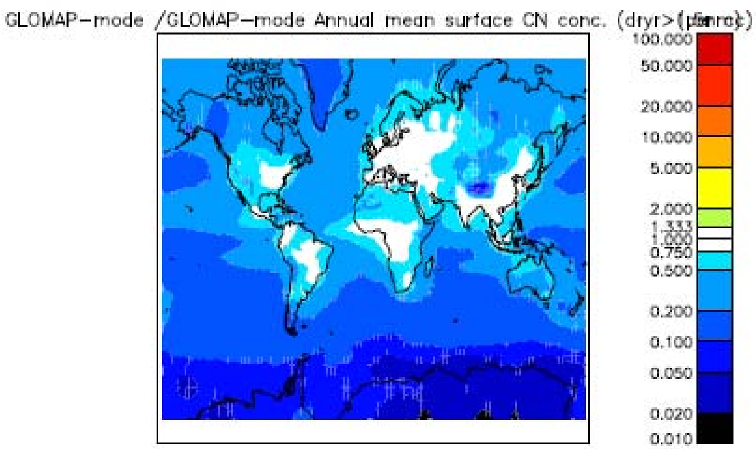
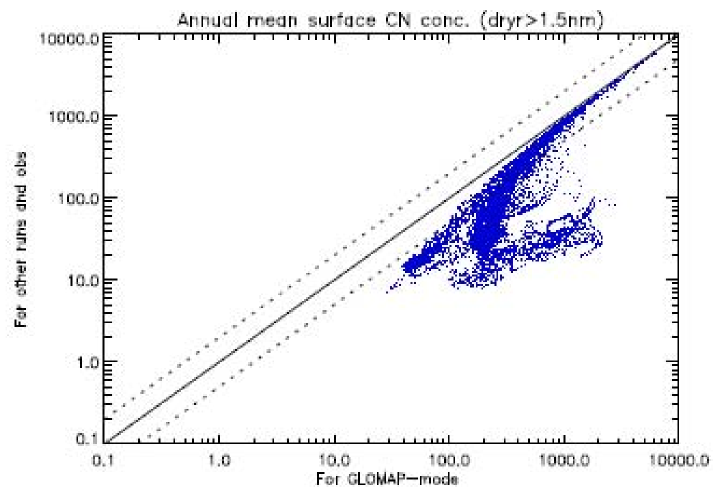




A2-SIZ4
2006
(nucleation
switched off)





Secondary aerosol particles > 50% of surface CN in almost all marine regions
Continental CN mostly from primary emissions (no BL nucleation in these runs).

CCN concentrations (GLOMAP-mode)

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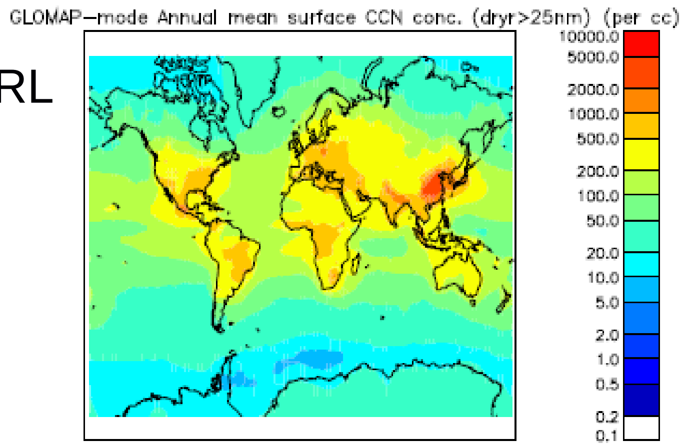
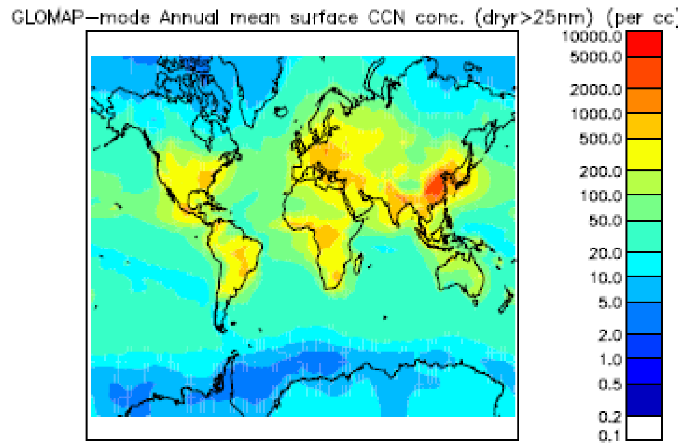
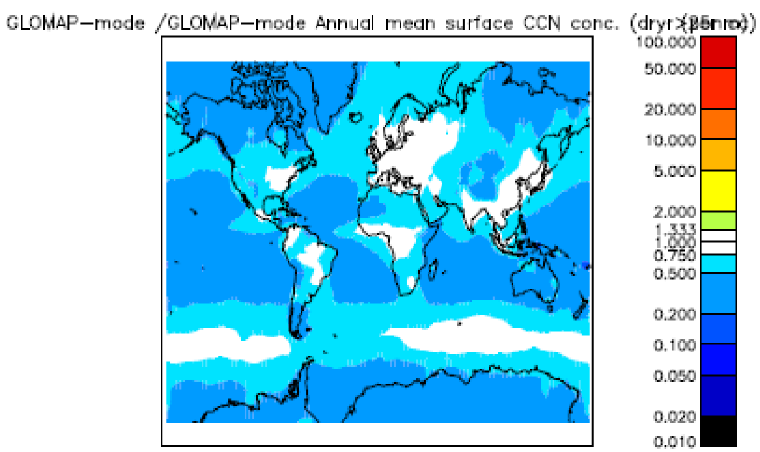
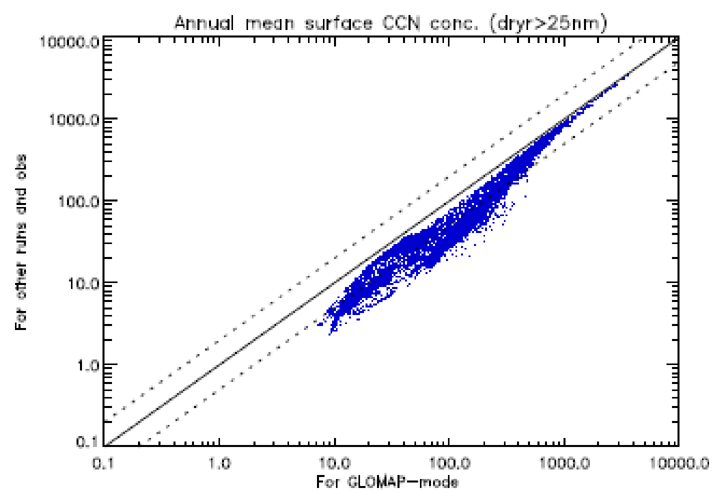
A2-CTRL
2006





A2-SIZ4
2006
(nucleation switched off)





30-50% surface CCN in most MBL regions from secondary aerosol
Sea-spray dominated regions and continental regions dominated by primaries.

SO4 mass concentrations (GLOMAP-mode)

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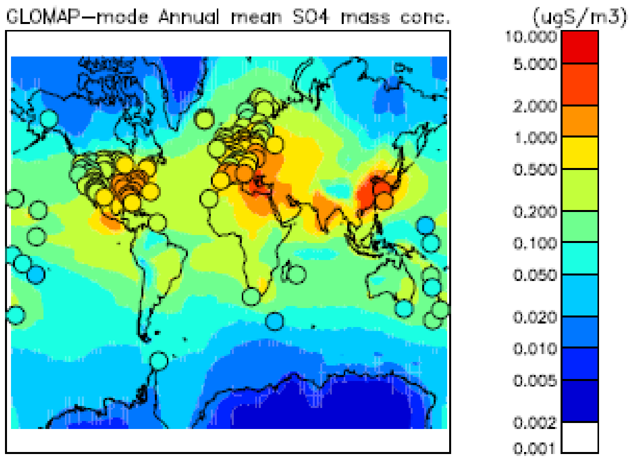
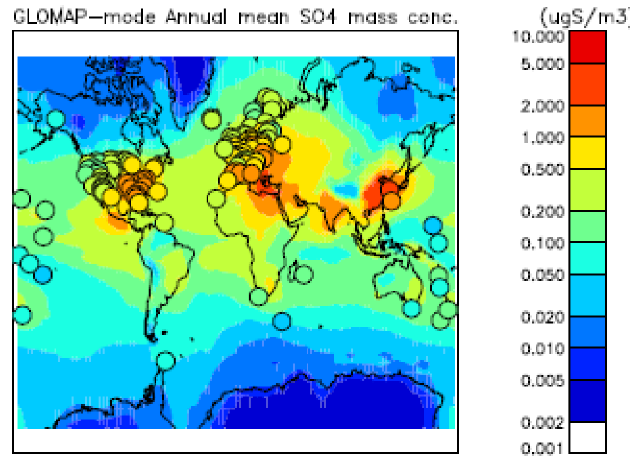
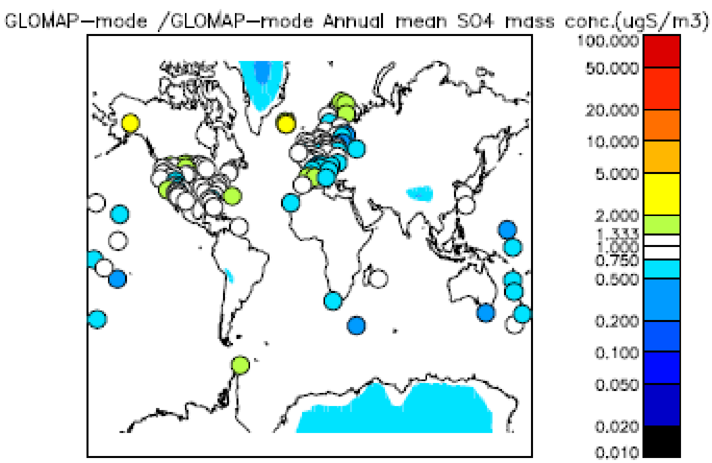
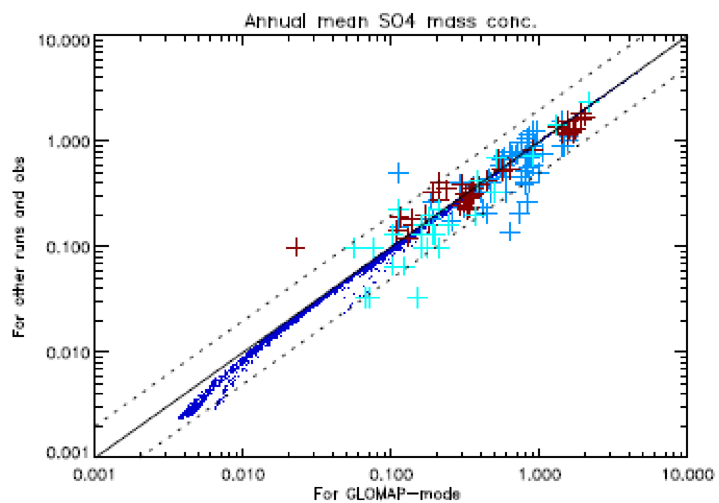
A2-CTRL 2006





A2-SIZ4 2006 (nucleation switched off)





Switching off nucleation makes no difference to simulated mass concentrations

CCN concentrations (GLOMAP-mode)

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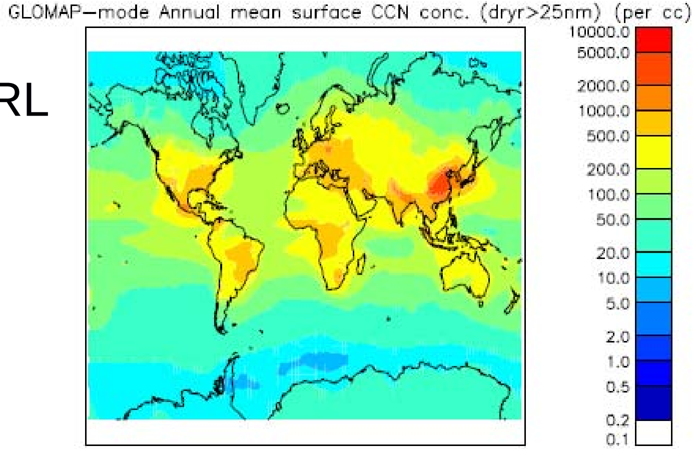
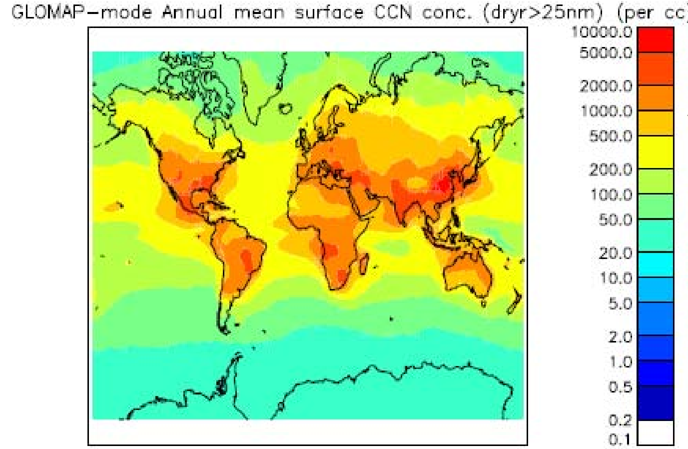
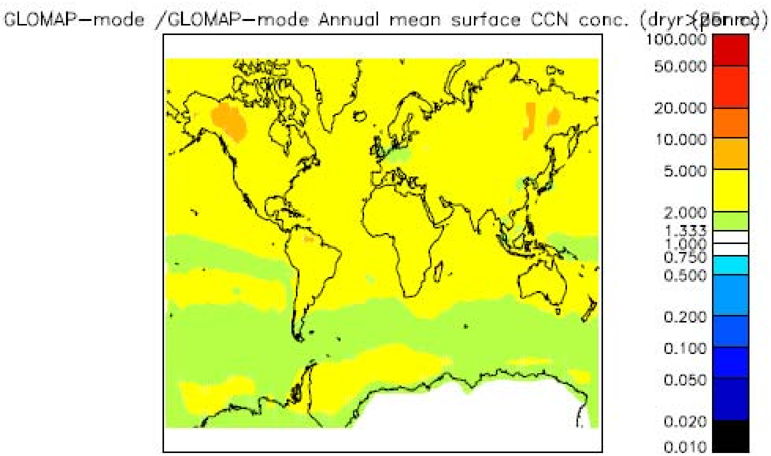
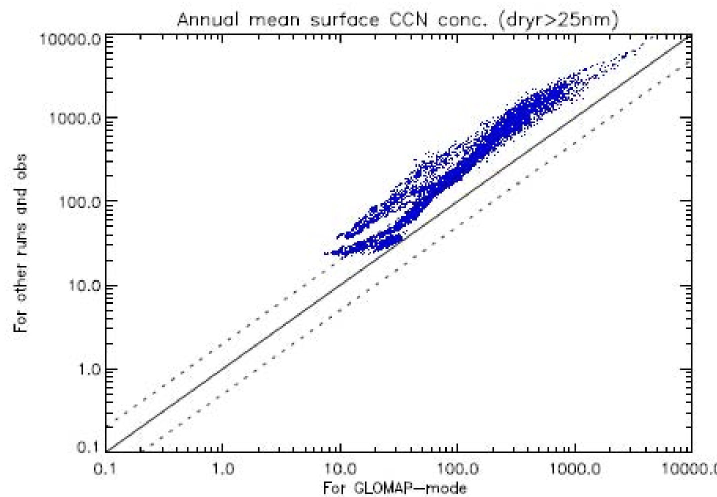
A2-CTRL
2006





A2-SIZ2
2006
(coagulation
switched off)





Switching coagulation off increases CCN concentrations by > 100%.

CN concentrations (GLOMAP-mode)

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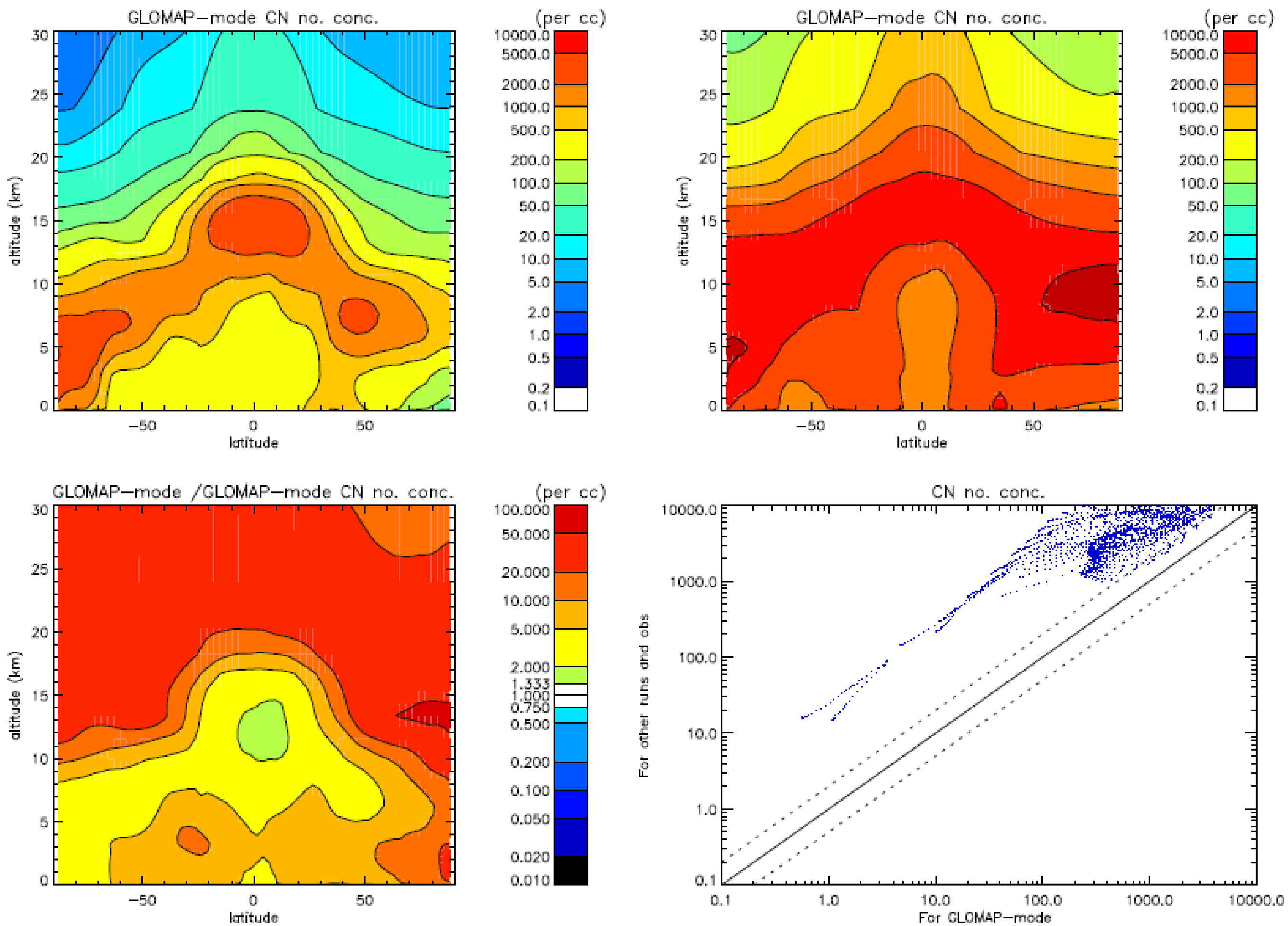
A2-CTRL
2006



A2-SIZ4
2006
(nucleation switched off)

Switching coagulation off strengthens observed CN peak in Upper Troposphere
Increases CN concentrations everywhere by ~ factor 2-10

Sites with CN observations over several years

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Station Name	Location	Altitude (m)	Observation period	Min. cutoff diameter (nm)	Reference
			Free troposphere		
Jungfraujoch	8.0E , 46.6N	3580	1995-1999, 2003-2007	10	Weingartner et al. (1999)
Puy de Dome	3.0E, 45.8N	1465	2005-2008	3	Venzac et al. (2009)
Nepal C.O.	86.8E, 28.0N	5079	2007-2008	10	Venzac et al. (2008)
Mauna Loa	155.6W, 19.5N	3397	1975-2000	10	Bodhaine (1996)
South Pole	24.8W, 90S	2841	1974-1999	10	
Pico Espejo	71.1W, 8.5N	4775	2007-2009	10	
Mount Washnigton	71.3W, 44.3N	1910	2002-2005	10	
			Marine boundary layer		
Mace Head	350.1E, 53.3N	0	2000, 2002-2007	10	O'Dowd et al. (1998)
Neumayer	8.3W, 70.7S	42	1993-2006	10	Weller and Lampert (2008)
Point Barrow	156.6W, 71.3N	11	1994-2007	10	Bodhaine (1989)
Samoa	170.6W, 14.2S	77	1977-2006	10	
Trinadad Head	124.2W, 41.1N	107	2002-2007	10	
Cape Grim	144.7E, 40.6S	94	1996-2007	3	Gras (1995)
Sable Island	60.0W 43.9N	5	1992-2000	10	

Spracklen et al, (2009, in preparation)

Sites with CN observations over several years

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Station Name	Location	Altitude (m)	Observation period	Min. cutoff diameter (nm)	Reference
			Continental boundary later		
Hyyti¨al¨a	24.3E, 61.9N	180.	2000-2004	3	Aalto et al. (2001)
Pallas	24.1E, 68.0N	340.	2000-2004, 2007	10	Komppula et al. (2003)
Finokalia	25.7E, 35.3N	0	1997, 2006-2007	10	
Hohenpeissenberg	11.0E, 47.8N	995	2006-2007	3	Birmili et al. (2003)
Melpitz	12.3E, 51.2N	86	1996-1997, 2003	3	
Bondville	88.4W, 40.1N	213	1994-2007	10	
Southern Great Plains	97.5W, 36.6N	320	1996-2007	10	
Tomsk	85.1E, 56.5N		2005-2006	3	Dal Maso et al. (2008b)
Listvyanka	104.9E, 51.9N		2005-2006	3	Dal Maso et al. (2008b)
Harwell	359.0E, 51.0N	60	2000	10	
Weybourne	1.1, 53.0N	0	2005		
Botsalano	25.8E, 25.5S	1424	7/2006-6/2007	10	Laakso et al. (2008)
India Himilaya	79.6E, 29.4N	2180	2005-2008	10	Komppula et al. (2009)
Aspvreten	17.4E, 58.8N	25	2000-2006	10	Dal Maso et al. (2008a)
Ut¨o	21.4E, 59.8N	8	2003-2006	7	Dal Maso et al. (2008a)
Varri¨o	29.6E, 67.8N	400	1998-2006	8	Dal Maso et al. (2008a)
Thompson Farm	289.1E, 43.1N	75	2001-2009	7	Ziemba et al. (2007)
Castle Springs	71.3W, 43.7N	406	2001-2008	7	

Sites with CN observations over several years

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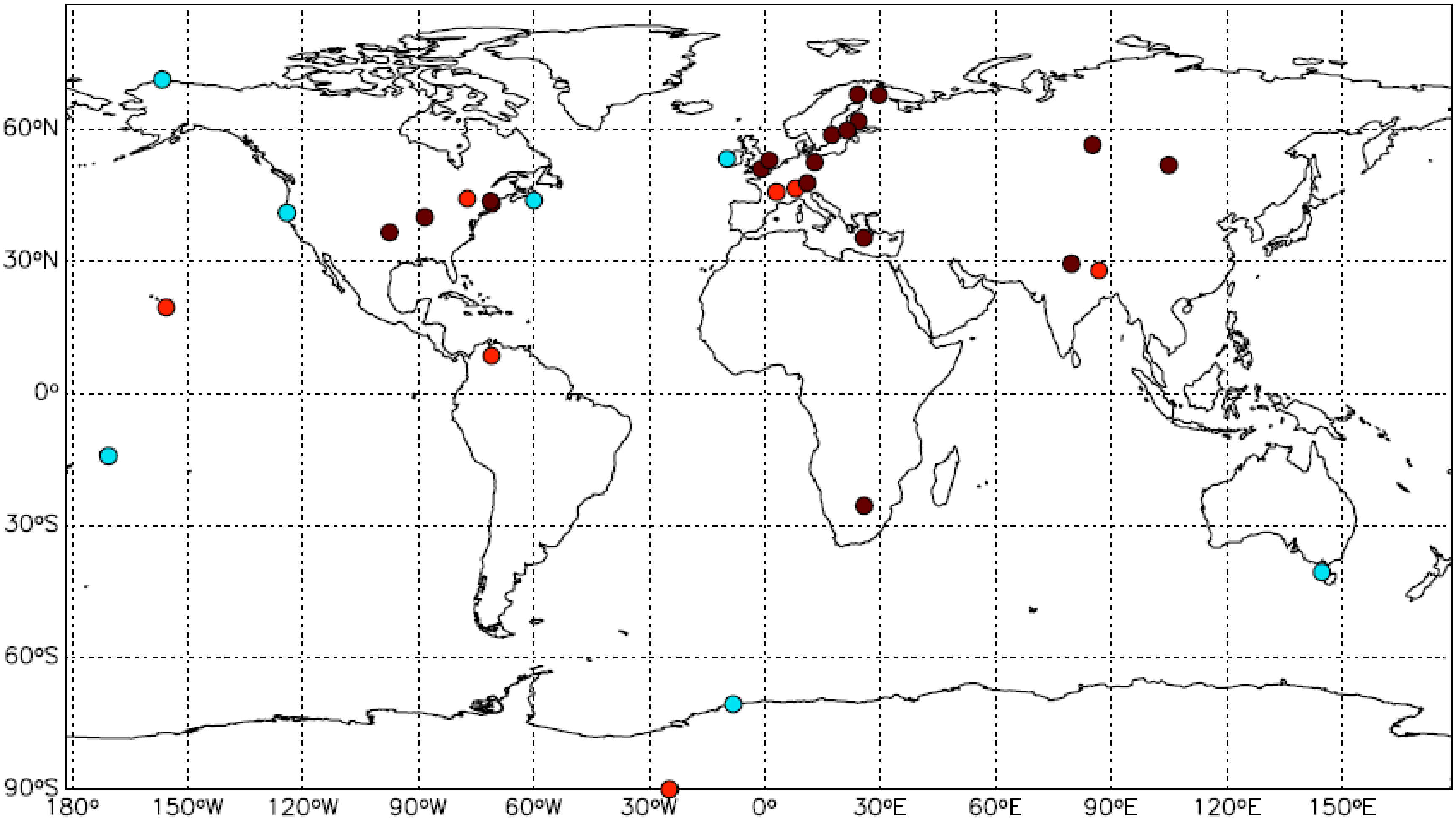

Remote marine BL sites

Continental BL sites

Free Troposphere sites

GLOMAP CN being evaluated against observations at GAW and ARM sites

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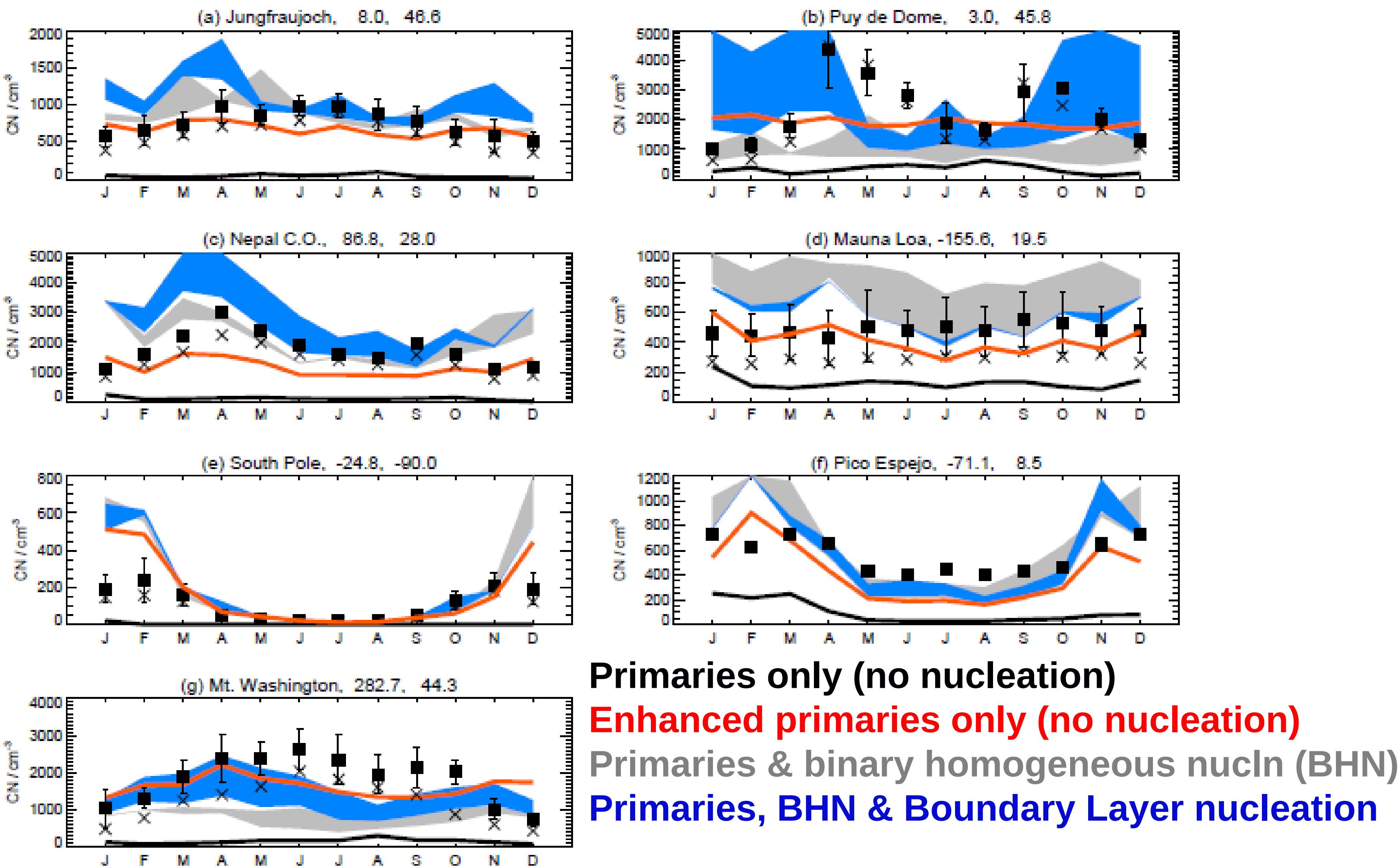

Spracklen et al, (2009, in preparation)

GLOMAP CN being evaluated against observations at GAW and ARM sites

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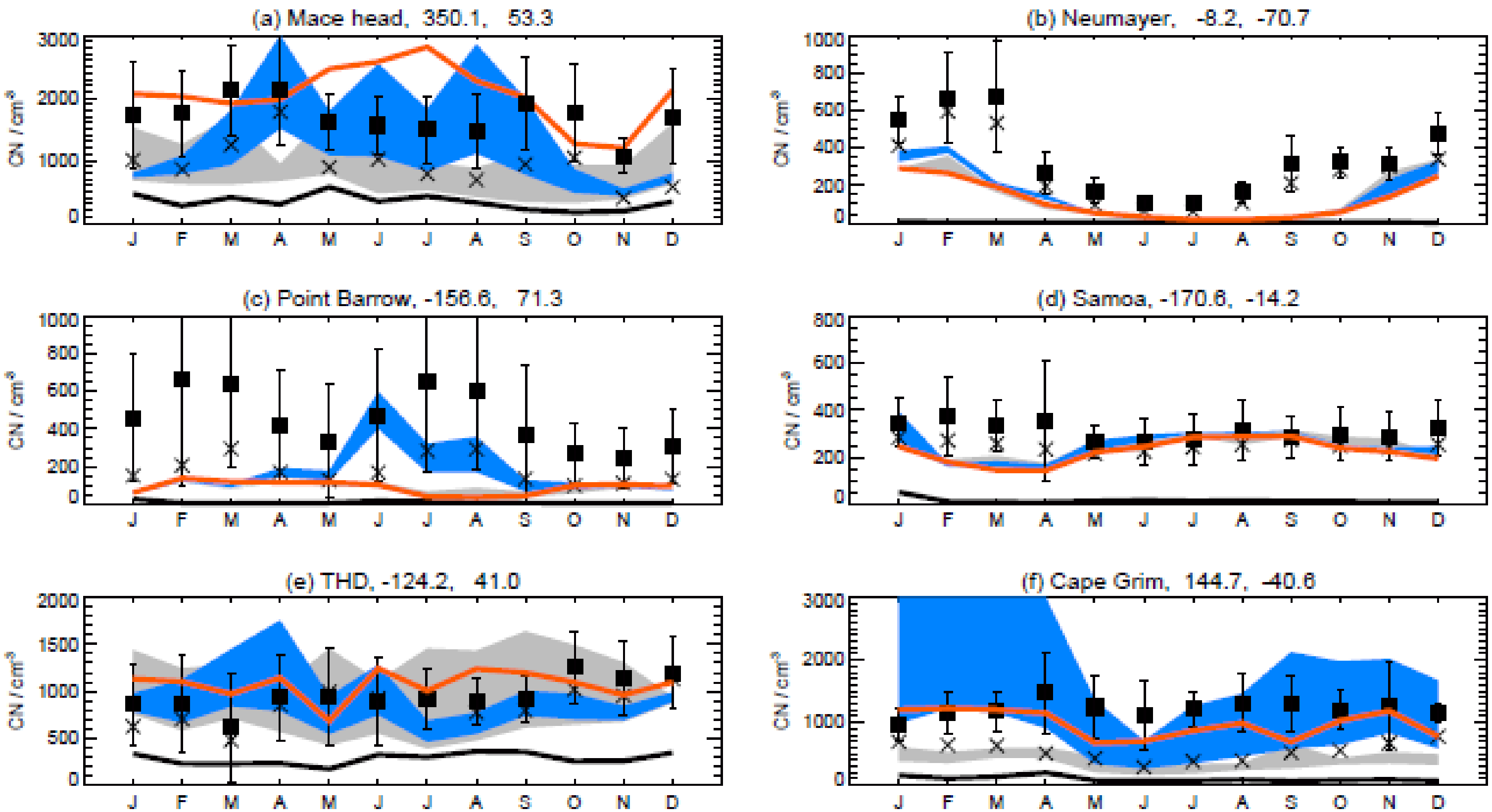

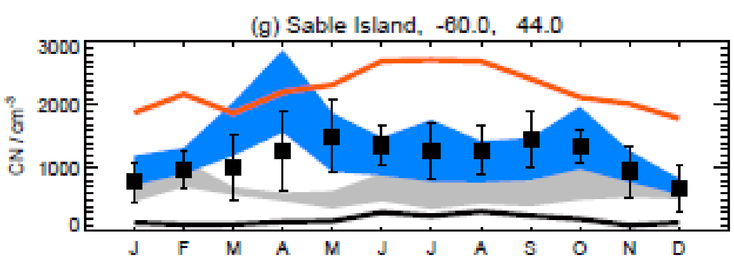

Primaries only (no nucleation)

Enhanced primaries only (no nucleation)

Primaries & binary homogeneous nucln (BHN)

Primaries, BHN & Boundary Layer nucleation

Spracklen et al, (2009, in preparation)

GLOMAP CCN being evaluated against a range of worldwide observations

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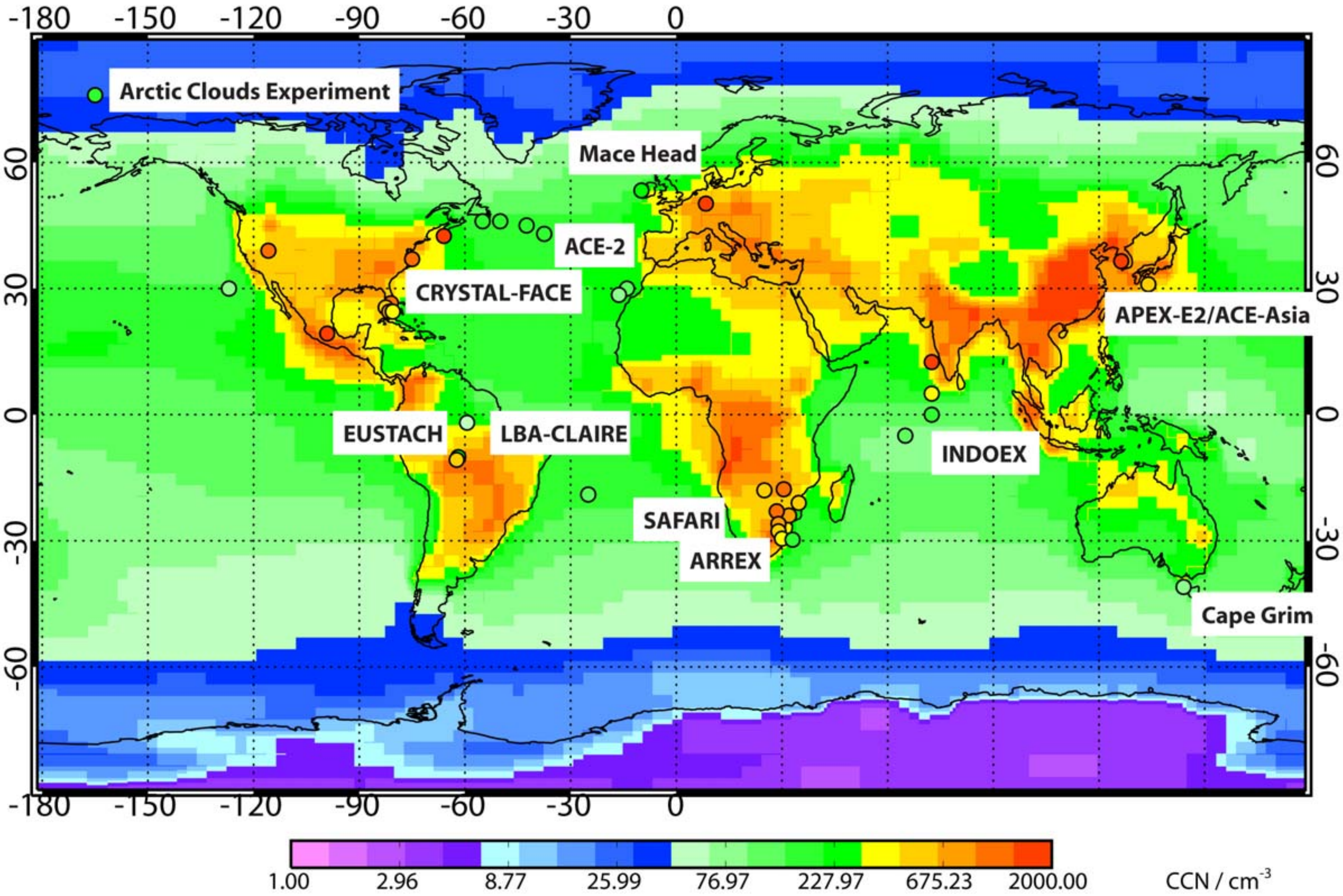

Note: map shows CCN at 0.2% supersaturations.
Coloured circles show observations at range of supersaturations

GLOMAP CCN being evaluated against a range of worldwide observations

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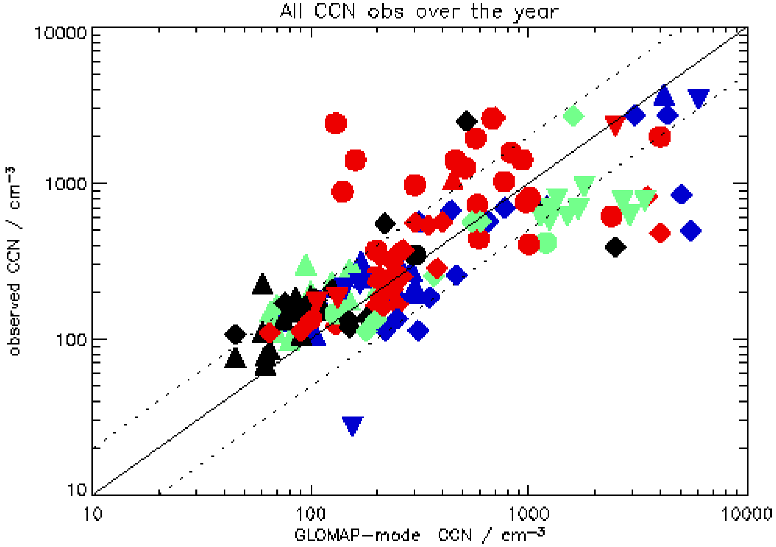
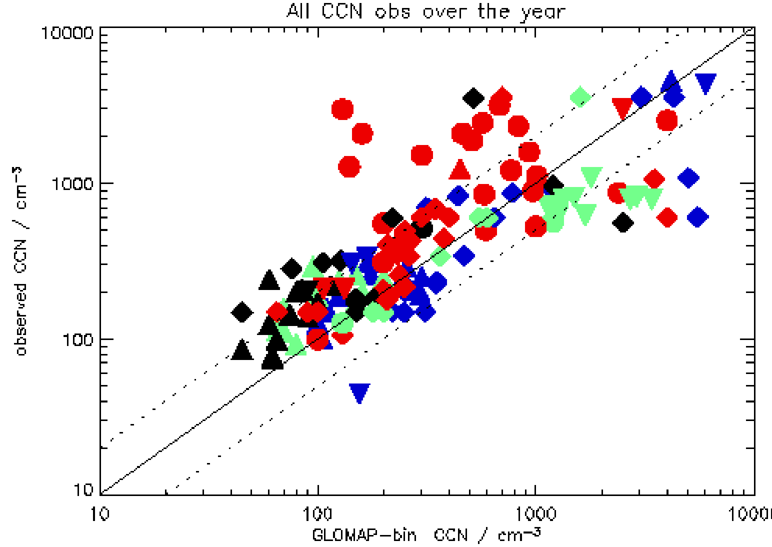
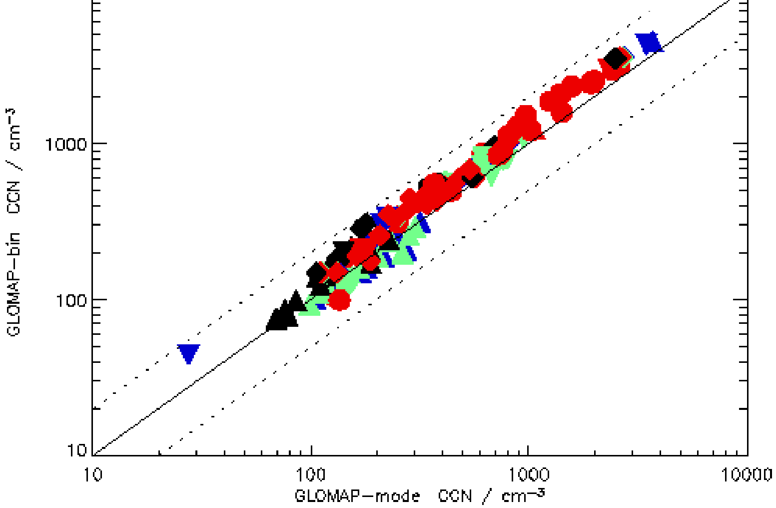
GLOMAP-mode vs. observations

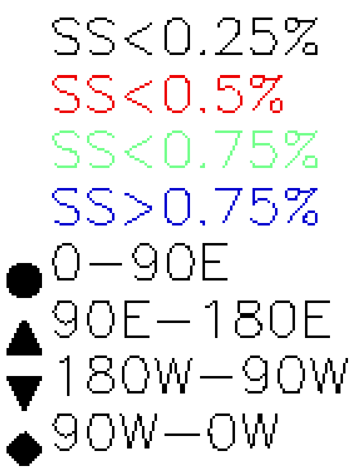


GLOMAP-bin vs. observations



GLOMAP-bin vs. -mode





GLOMAP size distributions being evaluated vs DMPS observations European EUSAAR supersites

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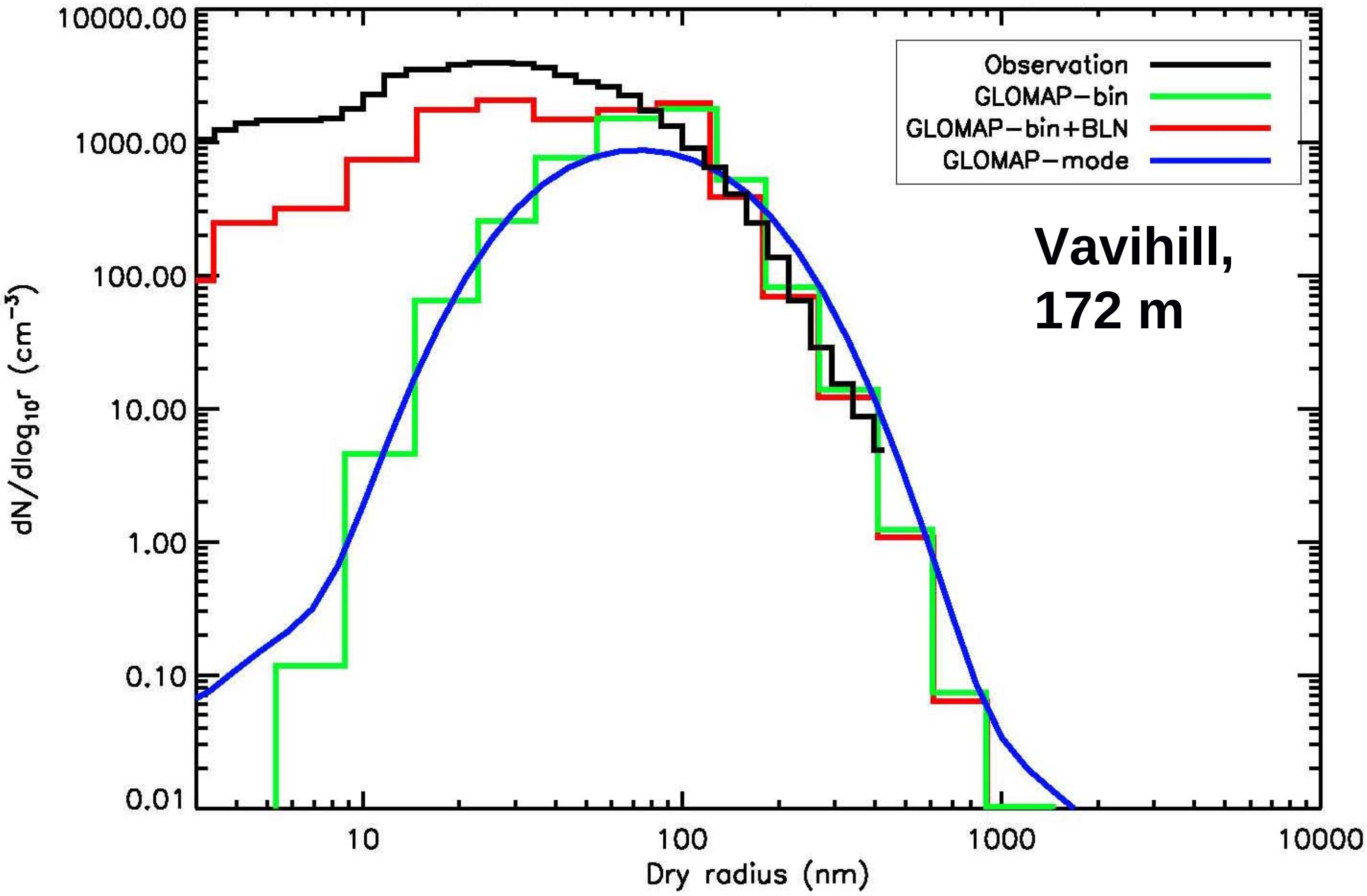

See poster by Maria Frontoso and Carly Reddington (University of Leeds)

GLOMAP size distributions being evaluated vs DMPS observations European EUSAAR supersites

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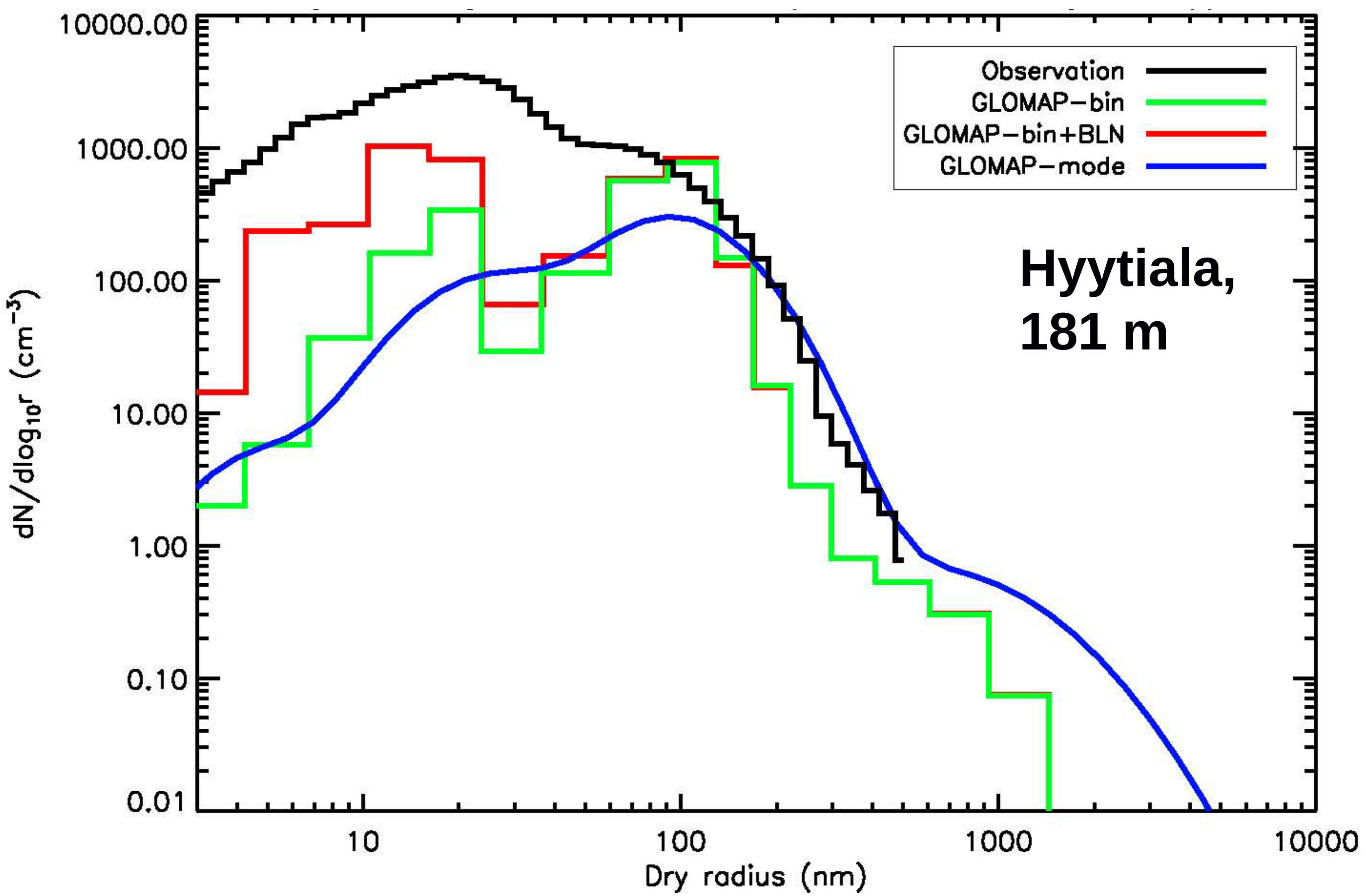

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GLOMAP being evaluated EUCAARI observations

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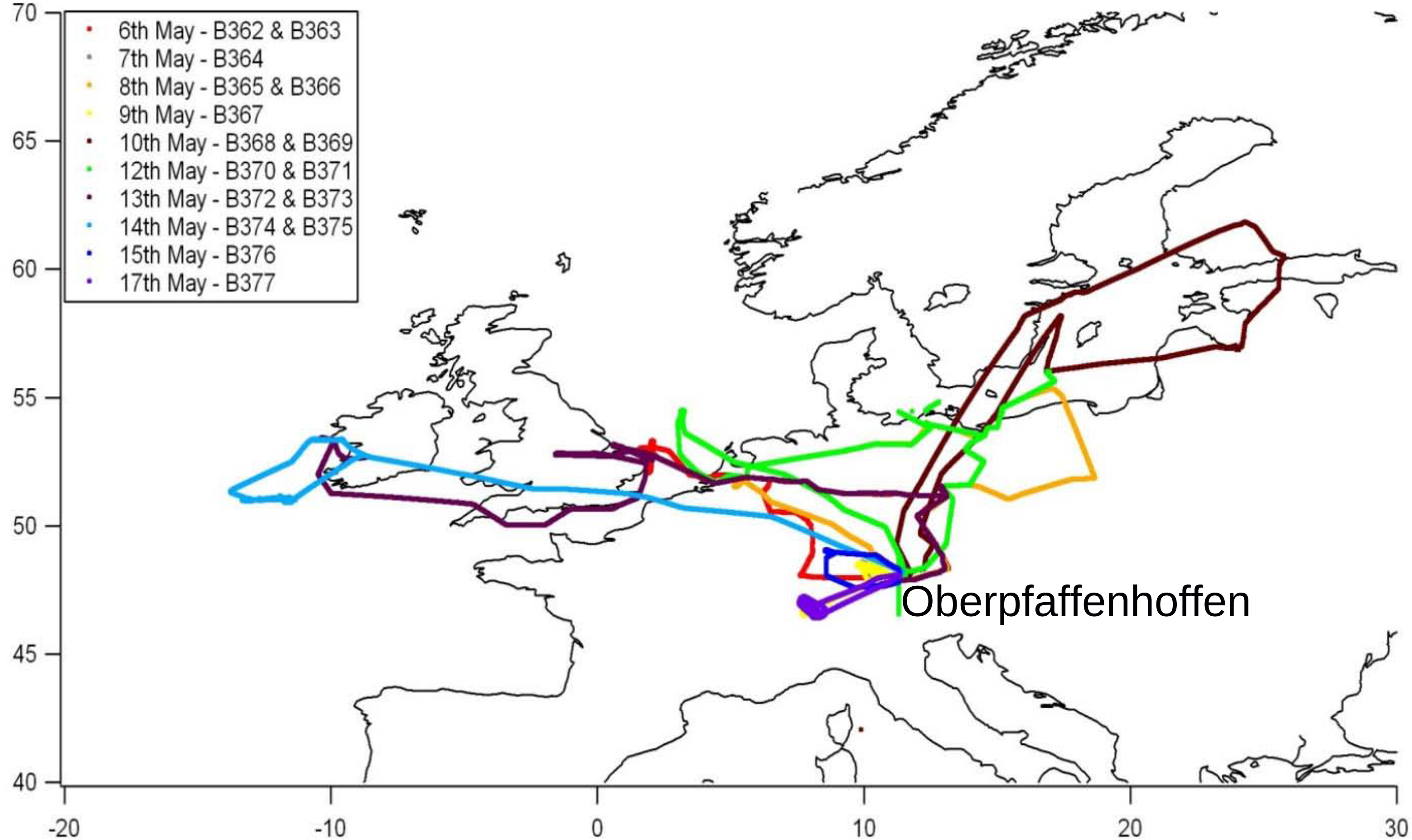
May 2008 EUCAARI-LONGREX flights – track evolution of aerosol properties over Europe (N-S and E-W transects)
(DLR Falcon, UK FAAM BAe146)



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GLOMAP being evaluated EUCAARI observations

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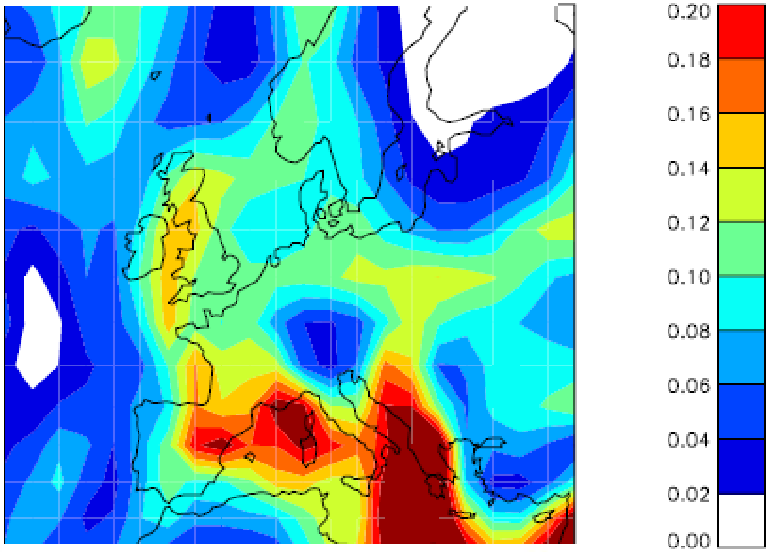
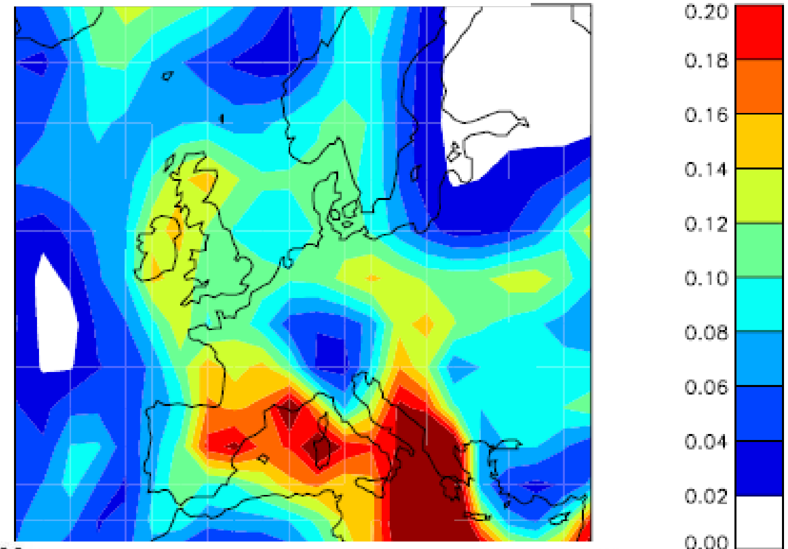
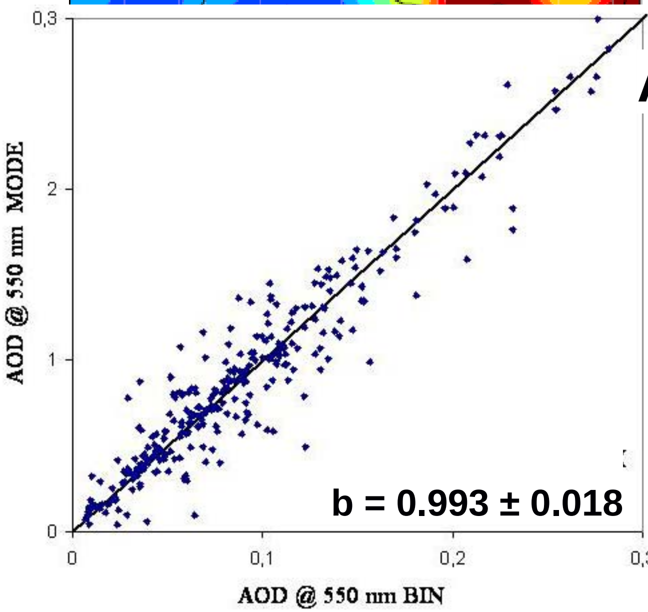
GLOMAP bin

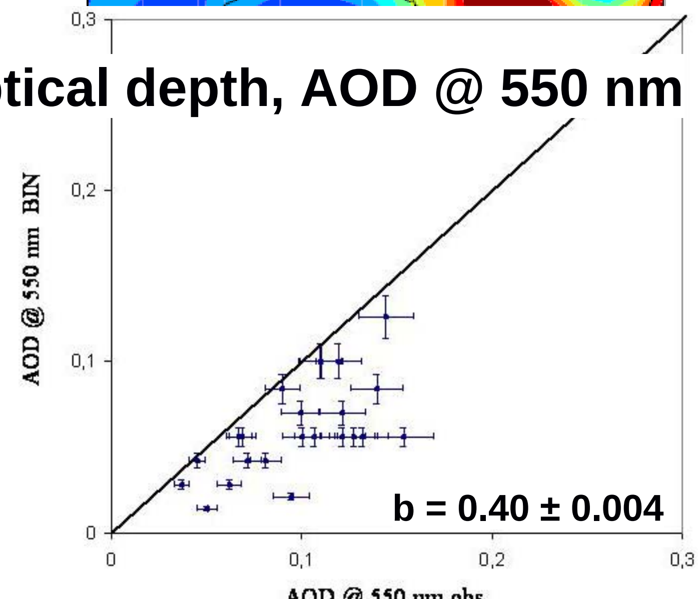


GLOMAP mode



Aerosol optical depth, AOD @ 550 nm





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GLOMAP being evaluated EUCAARI observations

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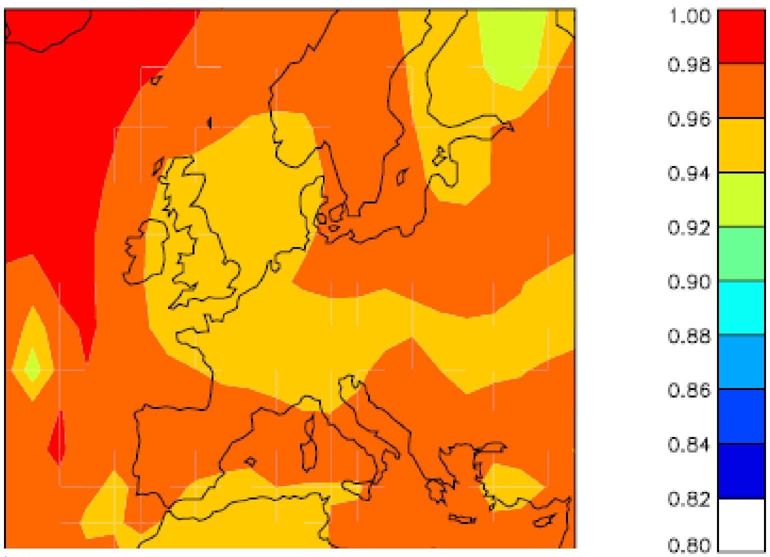
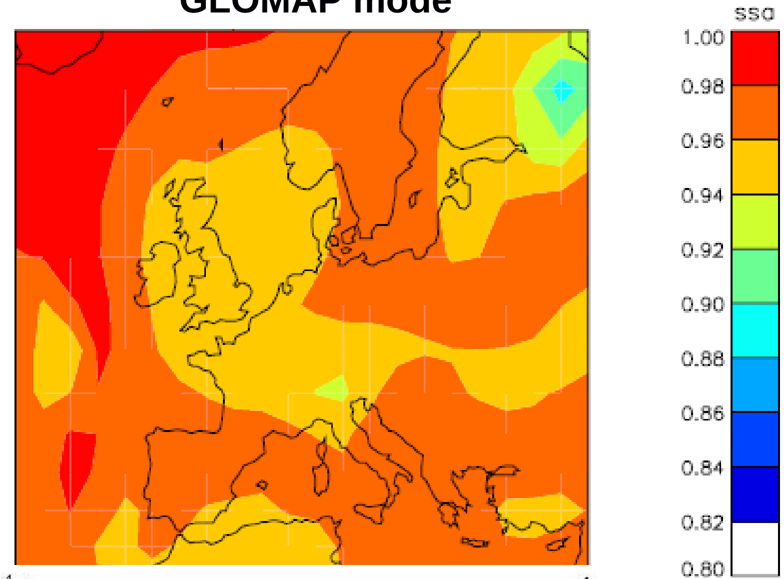
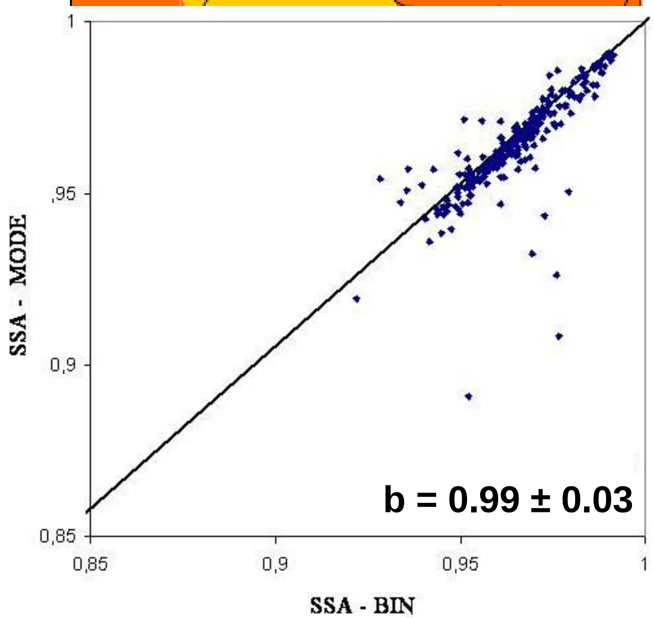
GLOMAP bin

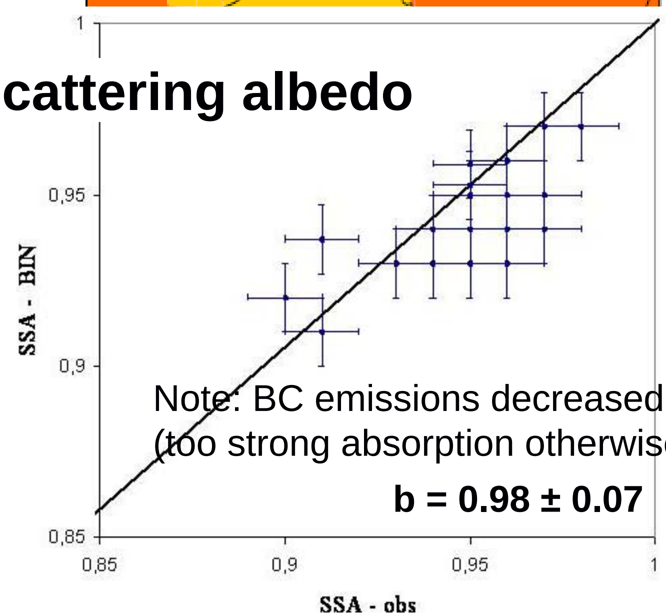


GLOMAP mode





Single scattering albedo



Note: BC emissions decreased by factor 3 (too strong absorption otherwise)

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AEROS Aerosol Model Uncertainty project

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Aerosol Model Robustness and Sensitivity study for improved climate and air quality predictions

3y Leeds/Oxford NERC project 2010-2012

- Develop techniques for sensitivity and uncertainty analysis of complex aerosol models (structural and parametric uncertainty)
- Quantify the most important factors controlling prediction diversity and biases against observations
- Evaluate models against synthesised aircraft, ground and remote observations from recent campaigns
- Define an appropriate level of model complexity and *enable future model development to be prioritised.*

Close collaboration with the Met Office and AEROCOM

Establish links with MUCM project

GLOMAP, UKCA and ECHAM-HAM models

Summary

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Original timeline for microphysics has slipped, but plan still the same.
-- Please submit your model's conccnxx and mmrtryy files to the AEROCOM server on 3D-M, 1D-D, 0D-H – use CMOR tables on website.
-- Please also provide your model's README file with instructions with order of aerosol tracers & how to calculate size distribution from your model tracers.

All-aerosol-tracer 3D-M, 1D-D, 0D-H data for GLOMAP-mode submitted to AEROCOM data server for A2-CTRL-2006 simulation
-- Please copy your models files over with A2-CTRL-2006 as soon as possible.

Assembled range of CN and CCN datasets at Leeds – can make available to AEROCOM for data server (assuming data PIs happy with this).

Wide range of new size distribution datasets from EUCAARI and EUSAAR now becoming available to help constrain models

Will compare each A2-CTRL vs current set of "number observations" in Leeds.

Then start to document diversity in simulated influence of microphysics on CCN, AOD using model sensitivity simulations A2-SIZ1,SIZ2,SIZ3,SIZ4 by end 2009.

New project AEROS starting March 2010 to quantify sources of model uncertainty at process level using aircraft, ground, remote-sensed and satellite observations over EUCAARI and EMEP intensive periods.