Evaluation of tropospheric aerosol properties simulated by HadGEM-UKCA & TOMCAT-GLOMAPmode

National Centre for Atmospheric Science — NATURAL ENVIRONMENT RESEARCH COUNCIL
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1. Introduction to UKCA

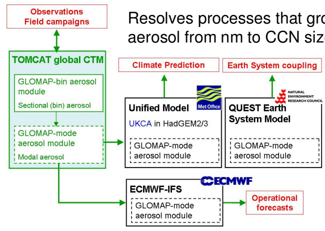
- Collaboration between NCAS & UK Met Office Hadley Centre since 2005. Universities of Leeds & Cambridge main NCAS partners
- Aerosol-chemistry sub-model in Met Office Unified Model environment for a range of applications (climate, Air Quality, Earth System science)
- Tropospheric and stratospheric chemistry schemes. Aerosol precursor extension to UKCA chemistry schemes so that climate model simulated aerosol is coupled to atmospheric chemistry.
- Improved representation of aerosol in UK climate model simulations
  -- new particle formation & growth using GLOMAP aerosol microphysics
  -- internally mixed aerosol (e.g. BC & sulphate) affect optical properties
  -- biogenic secondary organic aerosol from monoterpene oxidation
- UKCA interactive ozone, methane and aerosol (direct/indirect) radiative effects for fully coupled composition-climate simulations.
- Enhances UK capability in aerosol-climate-earth system modeling and provides integration for NCAS and Met Office initiatives.

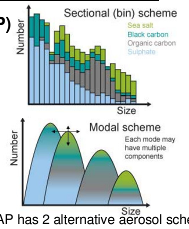
2. GLOMAP aerosol microphysics

Global Model of Aerosol Processes (GLOMAP)

Developed in Leeds since 2003 to simulate global aerosol with size-resolved number andcomposition.

Resolves processes that grow aerosol from nm to CCN sizes.



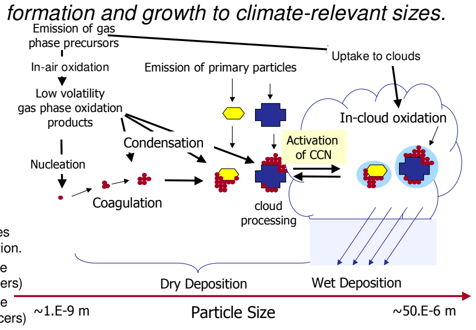


GLOMAP has 2 alternative aerosol schemes using the same/similar process representation.

GLOMAP-mode = 2-moment modal scheme (Mann et al, 2010) (~15-30 aerosol tracers)

GLOMAP-bin – 2-moment sectional scheme (Spracklen et al, 2005) (60-250 aerosol tracers)

Simulates aerosol lifecycle resolving new particle formation and growth to climate-relevant sizes.



4. UKCA chemistry schemes

A. Preliminary tropospheric scheme "Standard Tropospheric" (StdTrop):
8 emitted species, 46 species (26 advected), 129 reactions (27 are photolysis)
Simulates O_x, HO_x and NO_x chemistry with oxidation of CO, ethane & propane.
Aerchem Extension emits DMS, SO_2 & terpene species oxidation→ H_2SO_4 & SOA.
In-cloud oxidation of SO_2 to SO_4 via aqueous reaction with H_2O_2 and O_3.
Optional extra heterogeneous reactions based on online GLOMAP aerosol properties.

B. Stamdard tropospheric scheme "Trop chem with isoprene" (TropIsop):
9 emitted species, 55 species (48 advected), 164 reactions (35 are photolysis)
Same chemical cycles as above but additionally Mainz Isoprene Mechanism.
Aer-chem extension: As above but identical scheme to coupled TOMCAT-GLOMAP.
Optional extra heterogeneous reactions based on online GLOMAP aerosol properties.
Only gives biogenic SOA from monoterpenes → isoprene-derived SOA to be added.

C. Standard stratospheric scheme "StratChem/CheS"
Simpler tropospheric chemistry beneath more complex stratospheric scheme.
5 heterogeneous reactions based on UKCA-MODE surface area concentration.
Aer-chem extension: Stratospheric sulphur scheme with COS & photolysis reactions.

D. Whole-atmosphere chemistry scheme "WAChem/CheST"
Target supported chemistry which merges tropopheric and stratospheric chemistries
Aer-chem extension: merges TropIsop and Stratospheric aerosol chemistries.

Also **Extended Tropospheric Chem (ExtTC)** and **Regional AQ chem (RAQ)** schemes but these not yet coupled to GLOMAP-mode aerosol.

5. GLOMAP simulated aerosol in HadGEM-UKCA and in TOMCAT

Figure 1 : Dec & Jun DMS (surface)

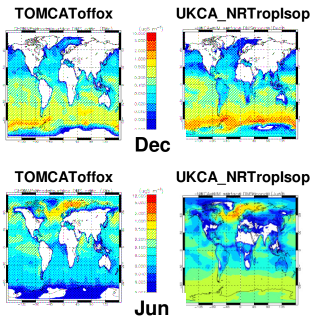


Figure 2 : Dec & Jun SO_2 (surface)

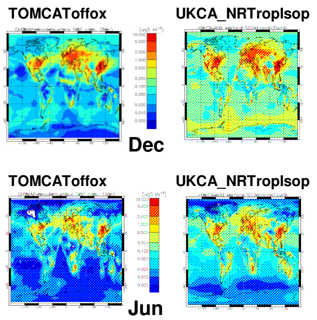


Figure 3 : Dec & Jun SO_4 (surface)

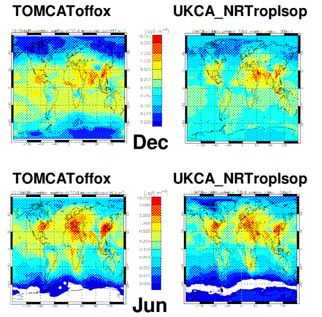


Fig 4 : Dec & Jun organic matter (srf)

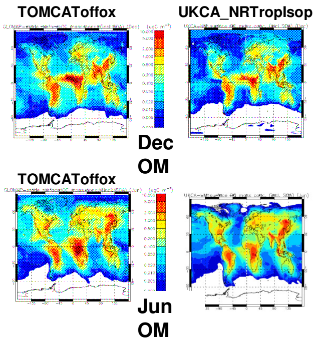


Fig 5 : EC & sea-salt (srf ann mean)

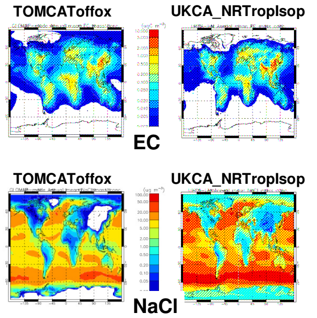


Fig 6 : CN_{10} & CCN_{70} (srf ann mean)

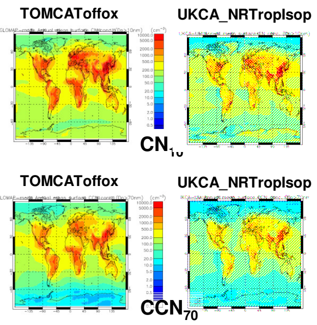
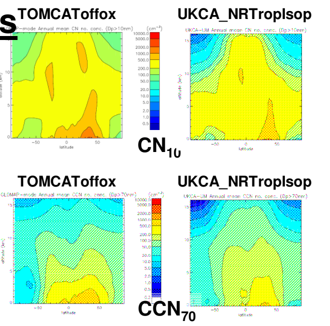


Fig 9 : CN_{10} & CCN_{70} (lat/alt, ann mean)



6. Runs used in comparison

Compare GLOMAP-mode simulated aerosol in HadGEM-UKCA against established TOMCAT-GLOMAP framework and observations.

TOMCAToffox T42L31 with 6-hrly monthly-mean oxidant fields (TOMCAT).
--- GLOMAP-mode v6 with revised modal settings as Mann et al . (2012)
--- AOD & forcings can be alculated offline based on monthly fields.
--- use AEROCOM phase 1 emissions (Dentener et al., 2006)

UKCA_NRTropIsop : N96L63 v7.3 HadGEM3-A-r2.0 TropIsop w FAST-J
--- GLOMAP-mode v6 with revised modal settings as Mann et al . (2012)
--- diagnose AOD & aerosol direct & indirect radiative effects online every radiation timestep using double-call to radiation scheme (RADAERv2)
--- use AEROCOM phase 2 emissions (Diehl et al., 2012)

UKCA_BEStdTrop : N96L38 v7.3 HadGEM3-A-prelim StdTrop w 2D-phot
--- GLOMAP-mode v5 with original modal settings as Mann et al . (2010)
--- diagnose AOD & aerosol direct & indirect radiative effects online every radiation timestep using double-call to radiation scheme (RADAERv1)
--- use AEROCOM phase 2 emissions (Diehl et al., 2012)

7. HadGEM-UKCA & TOMCAT-GLOMAP vs benchmark observational datasets

Fig. 7 : DJF & JJA AOD vs AERONET

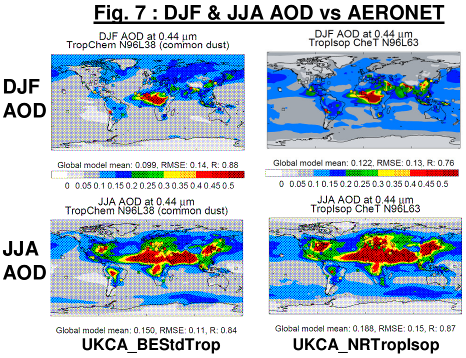


Fig. 8 : CCN vs compilation of observations (surf)

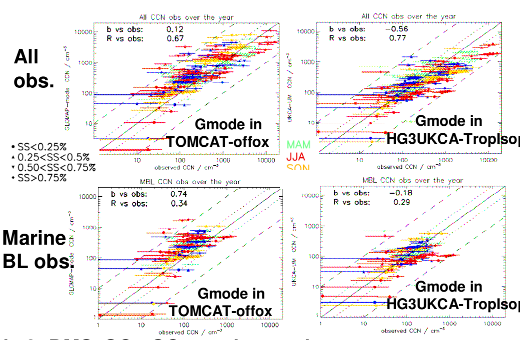


Fig 9 : CCN at Cape Grim

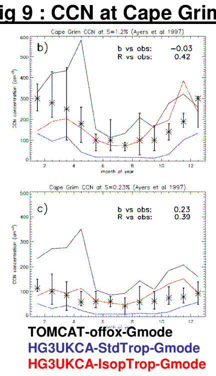


Table 1: Summary of burdens & production

Table 1. Annual mean global mass burden (Tg), emission fluxes, secondary production fluxes (both $Tg\,yr^{-1}$) for each aerosol component and the key precursor gases. The values for the 3 model runs: TOMCAT-Gmode, HG3-Gmode-BE-StdTrop and HG3-Gmode-NR-TropIsop are shown separated by commas in that order. Values in parentheses are the median value or range simulated by AEROCOM models as documented in Textor et al. (2006).

Species	Burden (Tg)	Prod (prim) ($Tg\,a^{-1}$)	Prod (sec) ($Tg\,a^{-1}$)
DMS	0.027, 0.099, 0.102 (0.02–0.15)	18.1, 14.3, 25.8 (10.7–23.7)	
SO_2	0.300, 0.477, 0.365 (0.2–0.68)	67.9, 58.6, 58.6 (64.4–104.1)	17.6, 14.3, 25.8 (15.9–24.7)
H_2SO_4	0.0001,0.0002,0.00004		10.8, 12.6, 24.5 (6.1–15.3)
MONOTER	0.0078,0.0345,0.0408	146.2, 128.6, 128.5 (127)	
SEC-ORG	0.0002,0.0002,0.00009		18.5, 14.7, 14.5 (7.1–42.9)
Sulphate	0.51 , 0.52 , 0.68 (0.66)	1.74, 0.753, 0.753 (59.6)	48.5, 46.3, 51.9
Sea-salt	3.39 , 2.03 , 8.12 (6.39)	2806, 3461., 3932. (6280)	
BC	0.100, 0.087, 0.109 (0.21)	7.72, 7.89 , 7.53 (11.3)	
POM	0.87 , 0.99 , 0.94 (1.21)	47.0, 51.3 , 36.6 (69.9)	26.0, 20.6, 20.3

Table 2: DMS, SO_2, SO_4 vs observations

Table 2. Simulated gas phase DMS and SO_2 against surface observations. Normalised mean bias (b) and Pearson correlation coefficient (R) are shown for each dataset. The values for the 3 model runs: TOMCAT-Gmode, HG3-Gmode-BE-StdTrop and HG3-Gmode-NR-TropIsop are shown separated by commas in that order. References for the observations are 1: Nguyen et al. (1992), 2: Ayers et al. (1991), 3: Jourdain and Legrand (2001) 4: Loevblad et al. (2004) 5: Holland et al. (1999) 6: Loevblad et al. (2004) 7: Malm et al. (2002) 8: from Stier et al. (2005).

Species	Site name	b	R	Ref.
DMS (ann. cycle)	Amsterdam I.	–0.43, –0.31, 0.11	0.72, 0.42, 0.35	1
DMS (ann. cycle)	Cape Grim	0.17 , 1.65 , 2.61	0.65, 0.77, 0.73	2
DMS (ann. cycle)	D. D'Urville	–0.43, 2.47 , 1.93	0.62, 0.73, 0.79	3
SO_2 (ann. cycle)	Amsterdam I.	–0.49, 0.16 , 1.57	0.64, 0.32, 0.50	1
SO_2 (ann. cycle)	Cape Grim	3.82, 9.83 , 19.14	0.47, 0.72, 0.72	2
SO_4 (annual)	Global marine	0.08, –0.69, –0.33	0.98, 0.89, 0.87	8
SO_2 (Dec)	Europe	1.12, –0.31, 1.34	0.61, 0.66, 0.65	4
SO_4 (Dec)	Europe	–0.70, –0.89, –0.76	0.63, 0.43, 0.60	6
SO_2 (Dec)	N. America	–0.46, –0.73, –0.01	0.88, 0.65, 0.93	5
SO_4 (Dec)	N. America	–0.50, –0.79, –0.47	0.72, 0.71, 0.89	7
SO_2 (Jun)	Europe	0.84 , 0.74 , 1.33	0.57, 0.62, 0.53	4
SO_4 (Jun)	Europe	0.47 , –0.66, 0.19	0.60, 0.69, 0.56	6
SO_2 (Jun)	N. America	-0.05 , 0.25 , 0.45	0.79, 0.53, 0.78	5
SO_4 (Jun)	N. America	0.29 , –0.48, 0.26	0.94, 0.75, 0.84	7

Table 4: Size-resolved-N vs obs (srf)

Table 4. Simulated CN and size-resolved number concentrations at the surface against each of the benchmark observational datasets. Normalised mean bias (b) and Pearson correlation coefficient (R) are shown. The values for the 3 model runs: TOMCAT-Gmode, HG3-Gmode-BE-StdTrop and HG3-Gmode-NR-TropIsop are shown separated by commas in that order. References for the observations are 9: Heintzenberg et al. (2000), 12: World Data Centre for Aerosols webpage (http://wdca.jrc.it).

Property	Size-range	Location	b	R	Ref.
CN (ann. mean)	$D_p > 10$ nm	Glo. marine	–0.14, –0.74, –0.57	0.12, 0.07, 0.16	9
N_{Ait} (ann. mean)	D_p 10–100 nm	Glo. marine	–0.41, –0.84, –0.65	–0.26, –0.23, –0.20	9
N_{acc} (ann. mean)	$D_p > 100$ nm	Glo. marine	0.16, –0.75, –0.63	0.77, 0.63, 0.75	9
CN (ann. cycle)	$D_p > 10$ nm	JFJ (FT)	–0.40, –0.70, –0.31	0.23, 0.52, –0.10	12
CN (ann. cycle)	$D_p > 14$ nm	MLO (FT)	–0.19, –0.43, –0.24	–0.33, 0.14, –0.01	12
CN (ann. cycle)	$D_p > 14$ nm	SPO (FT)	0.28, –0.36, 0.50	0.77, 0.81, 0.95	12
CN (ann. cycle)	$D_p > 10$ nm	MHT (MBL)	–0.53, –0.94, –0.87	0.17, 0.19, 0.67	12
CN (ann. cycle)	$D_p > 14$ nm	NEU (MBL)	–0.76, –0.94, –0.83	0.74, 0.82, 0.82	12
CN (ann. cycle)	$D_p > 14$ nm	BRW (MBL)	–0.84, –0.95, –0.88	–0.24, –0.02, 0.16	12
CN (ann. cycle)	$D_p > 14$ nm	SMO (MBL)	–0.47, –0.60, –0.35	–0.43, 0.51, 0.80	12
CN (ann. cycle)	$D_p > 14$ nm	THD (MBL)	–0.02, –0.82, –0.71	0.37, 0.33, 0.30	12
CN (ann. cycle)	$D_p > 3$ nm	CGR (MBL)	–0.61, –0.93, –0.80	0.43, –0.46, –0.03	12
CN (ann. cycle)	$D_p > 10$ nm	SGP (CBL)	–0.43, –0.87, –0.79	0.47, 0.22, 0.03	12
CN (ann. cycle)	$D_p > 14$ nm	BND (CBL)	–0.36, –0.81, –0.62	0.00, –0.01, –0.20	12
CN (ann. cycle)	$D_p > 10$ nm	PAL (CBL)	–0.41, –0.90, –0.80	–0.60, –0.38, –0.44	12
CN (ann. cycle)	$D_p > 3$ nm	HOP (CBL)	–0.06, –0.80, –0.57	–0.02, 0.57, 0.62	12

Table 3: NaCl, BC & POM vs observations

Table 3. Simulated aerosol mass of sea-salt, BC and OC against surface observations for each of the benchmark observational datasets. Normalised mean bias (b) and Pearson correlation coefficient (R) are shown. The values for the 3 model runs: TOMCAT-Gmode, HG3-Gmode-BE-StdTrop and HG3-Gmode-NR-TropIsop are shown separated by commas in that order. References for the observations are 7: Malm et al. (2002) 8: from Stier et al. (2005).

Component	Sites	b	R	Ref.
NaCl (annual)	Global marine	–0.45, –0.39, 0.75	0.13, –0.02, 0.04	8
EC (Dec)	N. America	–0.52, –0.94, –0.71	0.41, 0.20 , 0.58	7
OC (Dec)	N. America	–0.81, –0.97, –0.88	0.43, 0.35 , 0.64	7
EC (Jun)	N. America	–0.51, –0.80, –0.66	0.69, 0.56 , 0.67	7
OC (Jun)	N. America	–0.46, –0.68, –0.59	0.84, 0.26 , 0.49	7

Table 5: Size-resolved-N vs obs. (profile)

Table 5. Simulated CN and size-resolved number concentrations in vertical profile against each of the benchmark observational datasets. Normalised mean bias (b) and Pearson correlation coefficient (R) are shown. The values for the 3 model runs: TOMCAT-Gmode, HG3-Gmode-BE-StdTrop and HG3-Gmode-NR-TropIsop are shown separated by commas in that order. References for the observations are 10: Clarke and Kapustin et al. (2002), 11: from Lauer et al. (2005).

Property	Size-range	Location	b	R	Ref.
CN (ann. mean)	$D_p > 3$ nm	N.H. marine	–0.08, –0.67, 0.31	0.85, 0.72, 0.71	10
CN (ann. mean)	$D_p > 3$ nm	Trop'l marine	–0.54, –0.62, 0.097	0.70, 0.67, 0.60	10
CN (ann. mean)	$D_p > 3$ nm	S.H. marine	–0.07, –0.71, 0.22	0.87, 0.89, 0.92	10
N_5 (ann. mean)	$D_p > 5$ nm	Germany	–0.42, –0.46, –0.37	0.90,–0.11,–0.16	11
N_{15} (ann. mean)	$D_p > 15$ nm	Germany	–0.31, –0.37, –0.71	0.93,–0.14, 0.84	11
N_{120} (ann. mean)	$D_p > 120$ nm	Germany	–0.26, –0.70, –0.59	0.99, 0.92, 0.98	11

8. Summary

UKCA aerosol-chemistry sub-model now well established within HadGEM and central to the UK Met Office strategy in climate, air quality, dust & for aerosol effects on Numerical Weather Prediction

The GLOMAP-mode aerosol module now fully integrated into the HadGEM-UKCA composition-climate model for aerosol direct & indirect forcings

Simulated aerosol properties compare favourably against TOMCAT-GLOMAP and a range of benchmark observational datasets.

9. Current UKCA papers

Bellouin et al. (2012) Impact of the modal aerosol scheme GLOMAP-mode on aerosol forcing in the Hadley Centre Global Environmental Model, ACPD, 12, 21437-21479.
Kipling et al. (in prep.) Constraints from vertically-resolved aircraft observatoins on aerosol processes in climate models
Mann et al. (in prep.) Evaluation of the new UKCA climate-composition model – Part 3: Tropospheric aerosol properties
O' Connor et al. (in prep.) Evaluation of the new UKCA climate-composition model – Part 2: Tropospheric chemistry
Savage et al. (2012), AQ modelling using the Met Office UM: model description & initial evaluation, GMDD, 5, 3131-3182.
Telford et al.(2012), Implementation of the Fast-JX photolysis scheme into the UKCA model, GMDD., 5, 3217-3260.
West et al. (in prep.) The importance of vertical velocity variability for estimates of the indirect aerosol effects.

10. Other References

Dentener et al. (2006), Atmos. Chem. Phys., 6, 4321-4344.
Diehl et al. (2012), A. C. P.. Discuss., 12, 24895-24954.
Mann et al. (2010), Geosci. Mod. Devel., 3, 519-551..
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Spracklen et al., (2005), Atmos. Chem. Phys., 5, 2227–2252.