SPECIAL PROJECT PROGRESS REPORT

Progress Reports should be 2 to 10 pages in length, depending on importance of the project. All the following mandatory information needs to be provided.

Reporting year
…………… July 2014 to June 2015 …………….……

Project Title:
……… Development and testing of a microphysical aerosol scheme in the IFS ……………………….……

Computer Project Account:
SPGBWOOD ………………………………………….……

Principal Investigator(s):
Dr. Graham Mann.……………………………………….…

……………………………………………………….………

Affiliation:
University of Leeds …………………………….……

Name of ECMWF scientist(s) collaborating to the project
(if applicable)
Jean-Jacques Morcrette, Johannes Flemming, Samuel Remy, Richard Engelen, Angela Benedetti.……

……………………………………………………….………

Start date of the project:
Jan 2015 (previous project ran Jan 2012 to Dec 2014)…

Expected end date:
Dec 2017………………………………………………….……

Computer resources allocated/used for the current year and the previous one
(if applicable)
Please answer for all project resources

		Previous year		Current year	
		Allocated	Used	Allocated	Used
High Performance Computing Facility	(units)	2,000,000	???	3,000,000	942,452 (at June15)
Data storage capacity	(Gbytes)	???	???	15,000	???

Summary of project objectives (10 lines max)

A new aerosol module "GLOMAP-mode" has been implemented into the IFS to upgrade on the mass-based scheme developed initially and referred to here as IFS-LMD (Morcrette et al., 2009). The GLOMAP-mode aerosol microphysics scheme (e.g. Mann et al., 2010; Mann et al., 2012) simulates the evolution of the particle size distribution, with explicit sources and sinks of particle number (e.g. via nucleation and coagulation) as well as mass. The scheme tracks the same component masses as the IFS-LMD scheme (sulphate, sea-salt, mineral dust and black and organic carbon) but calculates their composition across the size range resolving internal mixtures and gas to particle transfer. Resolving these aerosol microphysical processes has been shown to improve the fidelity of simulated aerosol radiative forcings (Bellouin et al., 2013) and provides improved aerosol boundary conditions to regional air quality models, many of which include similar aerosol microphysics schemes. In this 2nd phase of the IFS-GLOMAP special project (SPGBWOOD) the focus is on coupling the model to other aspects such as the sulphur cycle from the TM5 tropospheric chemistry scheme in C-IFS for a sulphate-coupled chemistry-aerosol-microphysics capability. This sulphate-coupled C-IFS-GLOMAP system will also be extended to also link up with the ammonia and nitric acid species already simulated in TM5, with the two semi-volatile gases then partitioning into each size mode using a new "dissolution module" for GLOMAP (Benduhn et al., 2015)…………………………………

Summary of problems encountered (if any) (20 lines max)

The main problem encountered so far has been in the implementation of dust within IFS-GLOMAP.

Dust is a core component of GLOMAP, with the insoluble accumulation and coarse modes receiving emissions of dust (see e.g. Mann et al., 2010) and, following uptake of soluble material, dust particles are "aged" across to the corresponding soluble mode where they are more efficiently scavenged.

However, at the time of the last SPGBWOOD progress report (July 2014), in IFS-GLOMAP runs the dust component of GLOMAP had to be de-activated because simulations at that time showed highly spurious features of very high dust concentrations in the regions of the Himalayas (several orders of magnitude too high) with subsequent propagation to the rest of the domain. For the assessments of simulated AOD in MACC-II deliverable report D62.3, dust AOD from a simulation with the GEMS/MACC aerosol scheme (fuw5 in cycle 38r2) had to be added to the IFS-GLOMAP AOD.

In June and July 2014 the source of the problems with the IFS-GLOMAP dust were investigated with test runs with additional diagnostics to probe the sources and sinks of dust at high temporal resolution. The test runs illustrated that the interactive dust emissions in GLOMAP were working but there was a corruption of the GLOMAP dust mass mixing ratios at the beginning of new forecast cycles, which was causing the spurious features and resulting in the delays with the development of the scheme.

Since the last SPGBWOOD progress report, the problems with dust in IFS-GLOMAP are entirely repaired. When the GLOMAP codebase was ported to cycle 40r3 in October 2014, Richard Engelen (ECMWF) discovered that indeed there was an over-write error that was causing the dust problems. That bug is now repaired and at 40r3 IFS-GLOMAP now simulates all species covered by IFS-LMD.

Summary of results of the current year (from July of previous yr to June of current year)

Substantial progress has been made on MACC-III deliverable D26.4 towards the implementation of the nitrate-extended GLOMAP system into C-IFS.

Firstly, the plan to implement a coupled aerosol-chemistry version of IFS-GLOMAP in C-IFS has been successfully carried out, with the sulphate production in GLOMAP being derived from the TM5 tropospheric chemistry module in C-IFS. Surface particulate sulphate concentrations simulated in "coupled aerosol-chemistry C-IFS-GLOMAP" have been evaluated against surface measurements from monitoring stations in Europe, North America and the North Atlantic,

comparing also to IFS-GLOMAP runs using the existing fixed-timescale SO_2 oxidation approach. Accurately characterising the seasonal cycle in sulphate is an essential first step towards accurately simulating nitrate aerosol variations because of the requirement of excess ammonia above that used up in the formation of ammonium sulphate.

As described in MACC-II Deliverable report D62.5, once this coupling of the sulphate production between TM5 and GLOMAP was completed, the plan was then to extend it to also couple TM5 simulated ammonia and nitric acid to a new "nitrate-extended" version of GLOMAP, the partitioning to the particle phase then occurring to the GLOMAP size-resolved ammonium (NH4) and nitrate (NO3) aerosol tracers, rather than to the single-tracer NO3 and NH4 aerosol in C-IFS.

Initial C-IFS-GLOMAP test runs have confirmed the successful implementation of the required extra aerosol tracers for nitrate-extended GLOMAP (as scoped in MACC-III deliverable D26.1). The additional FORTRAN subroutines required for nitrate-extended GLOMAP have also been added to a perforce branch in the IFS and compiled successfully.

Work to adapt the GLOMAP module to simulate stratospheric aerosol properties as well as tropospheric aerosol properties has continued with interactive stratospheric aerosol simulations with GLOMAP in the UK Met Office Unified Model (high top v7.3 N48L60 climate model). In particular the treatment of evaporation of sulphuric acid aerosol particles in the mid-stratosphere has been implemented and described in a paper published in ACP at the end of 2014 (Dhomse et al., 2014).

The stratospheric aerosol research has continued with these updates to GLOMAP also ported into an updated version of the v8.4 stratosphere-troposphere chemistry-aerosol-microphysics version (CheST+GLOMAP) of the UK Chemistry and Aerosol module, as released for use by researchers in the UK University community (see http://www.ukca.ac.uk/wiki/index.php/Release_Job_RJ4.0).

A recent additional development of the v8.4 UM-UKCA stratosphere-troposphere community composition-climate model has been the implementation of Meteoric Smoke Particles (MSP) in collaboration of the MACC-III Leeds researchers (Dr. Graham Mann, Dr. Sandip Dhomse) with other scientists at the University of Leeds (Prof. John Plane, Dr. James Brookes, Dr. Wuhu Feng) and the US National Centre for Atmospheric Research (NCAR, Boulder). The initiative has been part of an ERC project "Cosmic Dust in The Atmosphere" (CODITA) and has resulted in UM-UKCA now imposing MSP distribution in the upper stratosphere from the NCAR WACCM model to allow for MSP influences on stratospheric aerosol (e.g. Mills et al., 2005; Saunders et al., 2013).

Such interactions in the stratosphere between solid particles and sulphuric acid aerosol are also important to understand in relation to suggested Solar Radiation Management ideas which would involve injection of idealised particle with potential influence on ambient or volcanically enhanced stratospheric aerosol (e.g. Ferraro et al., 2011; Pope et al., 2012).

A PhD studentship at Leeds investigating data assimilation of gas phase and aerosol observations into the IFS has now completed two years (Tim Keslake, supervised by Martyn Chipperfield and Graham Mann at Leeds, ECMWF supervisor Johannes Flemming). The project examines the influence of biomass burning on atmospheric composition and has involved Tim running C-IFS and C-IFS-GLOMAP simulations with emissions from the GFAS fire module developed during MACC and MACC-II (e.g. Remy and Kaiser, 2014) to drive simulations with and without aerosol and chemistry data assimilation. Evaluation of case studies against aircraft and ground based measurements from the SAMBBA field campaign (e.g. Brito et al., 2014) have been carried out and analysis has continued to assess the improvement in model skill produced by using the data assimilation of aerosol and chemistry observations.

Finally, in this progress report we mention a recent development that is part of a collaboration between the University of Leeds and research scientists at CSIRO Aspendale, Australia. The collaboration has resulted in a new "lidar emulator" for GLOMAP being developed to derive attenuated backscatter profiles from the model, thereby retaining the full information on size-resolved aerosol composition as simulated in the model. The approach is a potentially powerful technique by which C-IFS with GLOMAP could provide an observational operator for satellite-borne lidar such as CALIPSO. MACC-III deliverable report D29.3 presents results from a case study demonstrating the potential new capability of the new GLOMAP lidar emulator comparing a transect of model derived 532nm total attenuated backscatter against that measured by CALIPSO for a satellite overpass crossing Australia during October 2006.

To allow more details of the findings towards the couplings of the TM5 atmospheric chemistry and the GLOMAP aerosol microphysics, and of the new GLOMAP lidar emulator, we have merged into this report the 3 deliverable reports carried out during MACC-III:

1) MACC-III Deliverable Report D26.1 (December 2014):
   "Configuration of extra tracers for nitrate-extended GLOMAP in IFS"

2) MACC-III Deliverable Report D62.4 (June 2015):
   "Test and evaluation of the "stand-alone" and "coupled to C-IFS" configurations of IFS-GLOMAP, the latter also with nitrate-extended GLOMAP"

3) MACC-III Deliverable Report D65.3 (June 2015):
   "Comparison of vertical profile and surface extinction coefficient against observations. (Lidar emulator for the GLOMAP aerosol microphysics module)".

SPGBWOOD users gb8 - Matthew Woodhouse   gbc - Martyn Paul Chipperfield
                gbi - Graham Mann   gbsd - Sandip Dhomse
                gbtk - Tim Keslake   gbwh - Will Hewson

List of publications/reports from the project with complete references

Description papers

- Dhomse, S. S., K. M. Emmerson. G. W. Mann, N. Bellouin, K. S. Carslaw, M. P. Chipperfield, R. Hommel, N. L. Abraham, P. Telford, P. Braesicke, M. Dalvi, C. E. Johnson, F. O'Connor, O. Morgenstern, J. A. Pyle, T. Deshler, and J. M. Zawodny, Whole-atmosphere aerosol microphysics simulations of the Mt Pinatubo eruption with the UKCA composition-climate model, *Atmos. Chem. Phys*, 14, 11221–11246, 2014.
- Mann, G.W., K.S. Carslaw, D.V. Spracklen, D.A. Ridley, P.T. Manktelow, M.P. Chipperfield, S.J. Pickering, and C.E. Johnson: Description and evaluation of GLOMAP-mode: a modal global aerosol microphysics model for the UKCA composition-climate model, Geosci. Model Dev., 3, 519-551, doi10.5194/gmd-3-519-2010.
- Mann, G. W., Carslaw, K. S., Ridley, D. A., Spracklen, D. V., Pringle, K. J., Merikanto, J., Korhonen, H., Schwarz, J. P., Lee, L. A., Manktelow, P. T., Woodhouse, M. T., Schmidt, A., Breider, T. J., Emmerson, K. M., Reddington, C. L., Chipperfield, M. P., and Pickering, S. J.: Intercomparison of modal and sectional aerosol microphysics representations within the same 3-D global chemical transport model, *Atmos. Chem. Phys.*, 12, 4449--4476, doi: 10.5194/acp-12-4449-2012, 2012.
- Remy, S. and Kaiser, J. W.: Daily global fire radiative power fields estimation from one or two MODIS instruments, *Atmos. Chem. Phys.,* 14, 13377–13390, 2014.

Other papers referred to in this report

- Bellouin, N., Mann, G. W., Woodhouse, M. T., Johnson, C. E., Carslaw, K. S., and Dalvi, M.: Impact of the modal aerosol scheme GLOMAP-mode on aerosol forcing in the Hadley Centre Global Environmental Model, *Atmos. Chem. Phys.*, 13, 3027-3044, doi:10.5194/acp-13-3027-2013, (2013).

- Benduhn, F., Carslaw, K.S., Pringle, K., Mann, G.W., Topping, D., McFiggans, G. et al: A Computationally Efficient Hybrid Solver of Inorganic Dissolution for Use in Global Models: I. Description, Validation and First Results., in prep., for submission to *Geosci. Mod. Dev.* (2015)

- Brito, J., Rizzo, L. V., Morgan, W. T., Coe, H., Johnson, B., Haywood, J., Longo, K., Freitas, S., Andreaea, M. O. and Artaxo, P.: Ground-based aerosol characterization during the South American Biomass Burning Analysis (SAMBBA) field experiment, *Atmos. Chem. Phys.*, 14, 12069–12083 (2014)

- Ferarro, A. J., Highwood, E. J., and Charlton-Perez, A. J.: Stratospheric heating by potential geoengineering aerosols, Geophys. Res. Lett., 38, L24706, doi:10.1029/2011GL049761 (2011).

- Mills, M. J., Toon, O. B., Vaida, V., Hintze, P. E., Kjaergaard, H. G., Schofield, D. P. and Robinson, T. W.: Photolysis of sulfuric acid vapor by visible light as a source of the polar stratospheric CN layer, J. Geophys. Res., 110, D08201, doi:10.1029/2004JD005519 (2005)

- Pope, F. D., Braesicke, P., Grainger, R. G., Kalberer, M., Watson, I. M., Davidson, P. J. and Cox, R. A.: Stratospheric aerosol particles and solar-radiation management, Nature Clim. Change, 2, 713-719.

- Saunders, R. W., Dhomse, S., Tian, W. S., Chipperfield, M. P., and Plane, J. M. C.: Interactions of meteoric smoke particles with sulphuric acid in the Earth's stratosphere, Atmos. Chem. Phys., 12, 4387–4398, 2012.

Summary of plans for the continuation of the project (10 lines max)

The Leeds research team are one of the partners in a proposal currently in progress responding to the "Development of Global Aerosol Aspects" Invitation To Tender within the current Copernicus Atmosphere Monitoring System (CAMS). If successful, the SPGBWOOD project will continue to support the testing and development of the IFS-GLOMAP and C-IFS-GLOMAP aerosol forecasting systems. In particular a major goal not yet complete from the MACC series of projects is the full coupling of the IFS-GLOMAP simulated aerosol properties with the AOD data assimilation system. With this coupling, it is anticipated that the IFS-GLOMAP system will replace the current operational IFS-LMD aerosol module over the next 2 years.

MACC-III Deliverable D26.1

Configuration of extra tracers for nitrate-extended GLOMAP in IFS

Work-package	Title
Deliverable	D26.1
Title	Configuration of extra tracers for nitrate-extended GLOMAP in IFS
Nature	R
Dissemination	Confidential
Lead Beneficiary	UNIVLEEDS (#32)
Date	12/2014
Status	Draft version
Authors	Graham Mann, Sandip Dhomse (Leeds, U.K.) Richard Engelen, Angela Benedetti (ECMWF) Francois Benduhn (Potsdam University, Germany)
Approved by	Olivier Boucher
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[In case the deliverable is not a report: provide a description of it inside this box.]

Executive Summary / Abstract

This brief report describes activities carried out to prepare for simulations in the IFS using a "nitrate-extended" version of the GLOMAP aerosol microphysics scheme to comprehensively track the evolution of the size-resolved inorganic composition of the particulate matter. The transition from the standard to the nitrate-extended version of GLOMAP is also occurring within the TOMCAT chemistry transport model and in the UM-UKCA composition-climate model frameworks. To accommodate the nitrate-extended GLOMAP, 12 additional tracers have been added, with the required the number of transported aerosol tracers increasing by 10 from 26 to 36. The extra composition information also required additional inputs to the RADAER module to be added, with also 12 extra "component partial volume" diagnostics added to the system.

Table of Contents

1. Introduction

During MACC, the GLOMAP aerosol microphysics module (Mann et al., 2010) was implemented into the IFS as an upgrade to the mass-based scheme (Morcrette et al., 2009) developed during GEMS. GLOMAP simulates the size-resolved evolution of the global aerosol, tracking particle number concentrations and the mass of sulphate, black carbon, organic matter, sea-salt and dust "components" within several size modes.

As part of MACC-II, the RADAER module (Bellouin et al., 2011) was added to the GLOMAP implementation within the IFS, to diagnose aerosol optical properties for each of the size modes, accounting for the simulated internally-mixed composition and size from the model. Also within MACC-II, the GLOMAP interfaces in the IFS were adapted to allow to run a fully integrated aerosol-chemistry configuration with GLOMAP coupled to the gas phase and aqueous phase SO2 oxidation calculated within the TM5 chemistry scheme within C-IFS.

In this MACC-III deliverable report, we describe work carried out to prepare for the upgrade of this chemistry-aerosol C-IFS-GLOMAP system to use a new "nitrate-extended" version of GLOMAP. This improved version of GLOMAP (Benduhn et al., 2014) has comprehensive treatment of the aerosol inorganic composition, with a substantial number of additional routines to accurately calculate size-resolved gas-to-particle partitioning of the semi-volatile gases nitric acid (HNO_3) and ammonia (NH_3) into nitrate and ammonium components in each soluble mode, together with the subsequent dissociation via aqueous phase equilibria. The nitrate-extended GLOMAP module no longer tracks a "sea-salt" component, instead separately tracking sodium and chloride masses in each mode, with an evolving aerosol pH and the potential to simulate degassing of HCl from the particle phase.

The main activity described here is the scoping to add the required additional tracers to the IFS and prepare for additional input variables for RADAER required from the nitrate-extended GLOMAP module, principally for the calculation of aerosol optical depths.

2. Overview of tracers needed for standard and nitrate-extended GLOMAP

In this section we give an overview of the current set of aerosol tracers used in the IFS-GLOMAP system, and present the additional tracers required for the extension to nitrate.

During December 2014, the Leeds MACC-III participants (G. Mann, S. Dhomse) visited ECMWF to discuss the requirements for the nitrate-extended scheme and assigned grib code numbers to use in future C-IFS-GLOMAP-nitrate simulations..

Figure 1 illustrates the current configuration of GLOMAP in the IFS, with the `gems_setup` script setting up 5 gas phase tracers being transported alongside the 26 aerosol tracers required by the microphysical scheme.   For the nitrate extension to GLOMAP, an additional 10 tracers are required (Figure 2) consisting of 8 for the nitrate and ammonium mass mixing ratios in each mode and the other two for the net of the 4 extra for sodium and chloride mass mixing ratios minus the two sea-salt tracers being replaced.

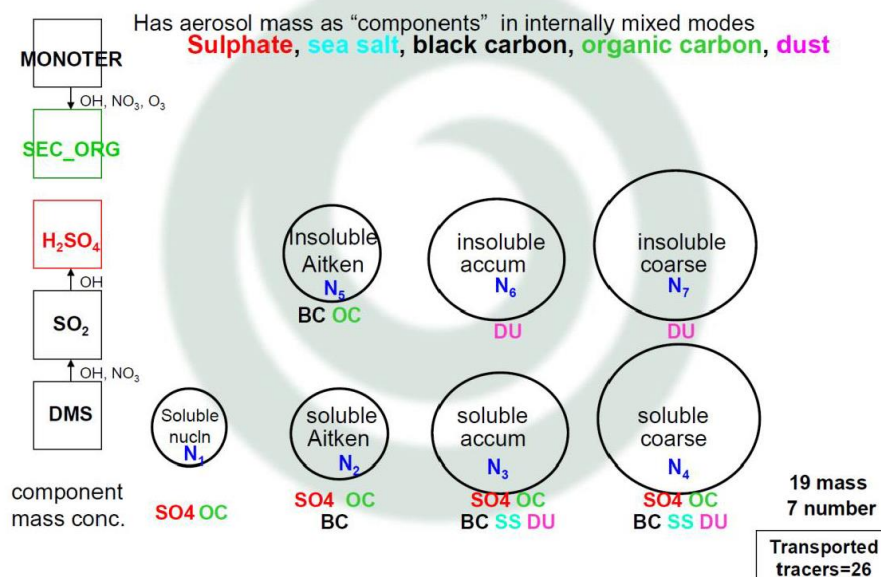## GLOMAP-mode standard config'n (with dust)

Figure 1. Standard configuration of GLOMAP within the IFS. There are 26 aerosol species consisting of 7 number mixing ratios (dark blue, N_i) and a total of 19 mass mixing ratios (**SO4, BC, OC, SS, DU** in each mode). 5 gas phase species (square boxes) are also provided.

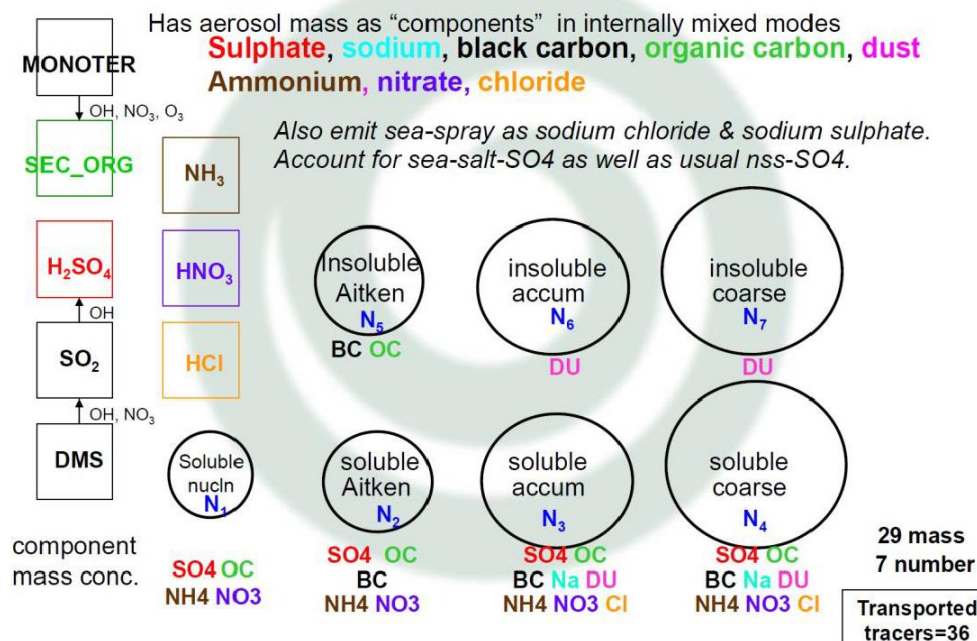## GLOMAP-mode extended config'n for nitrate

Figure 2. Nitrate-extended configuration of GLOMAP within the IFS. There are 36 aerosol species consisting of 7 number mixing ratios (dark blue, N_i) and a total of 29 mass mixing ratios (NH4, SO4, NO3, BC, OC, Na, Cl, DU in each mode). Note that here only the H2SO4, MONOTER and SEC_ORG gas phase tracers from GLOMAP are needed, with the TM5 chemistry module providing NH3 and HNO3 tracers together with SO2 aqueous and oxidation fluxes (accounting also for the source from DMS).

Item	Name of tracer (long name)	a	b	c
001	**Sulphate_NS** (mmr of SO4 in nucleation soluble mode)	X	X	X
002	**Sulphate_KS** (mmr of SO4 in Aitken soluble mode)	X	X	X
003	**Sulphate_AS** (mmr of SO4 in accumulation soluble mode)	X	X	X
004	**Sulphate_CS** (mmr of SO4 in coarse soluble mode)	X	X	X
005	**BlackCarb_KS** (mmr of BC in Aitken soluble mode)	X	X	X
006	**BlackCarb_AS** (mmr of BC in accumulation soluble mode)	X	X	X
007	**BlackCarb_CS** (mmr of BC in coarse soluble mode)	X	X	X
008	**BlackCarb_KI** (mmr of BC in Aitken insoluble mode)	X	X	X
009	**OrganCarb_KS** (mmr of OM in Aitken soluble mode)	X	X	X
010	**OrganCarb_AS** (mmr of OM in accumulation soluble mode)	X	X	X
011	**OrganCarb_CS** (mmr of OM in coarse soluble mode)	X	X	X
012	**OrganCarb_KI** (mmr of OM in Aitken insoluble mode)	X	X	X
013	**OrganCarb_NS** (mmr of OM in nucleation soluble mode)	X	X	X
014	**Sea-salt_AS** (mmr of SS in accumulation soluble mode)	X	X	
015	**Sea-salt_CS** (mmr of SS in coarse soluble mode)	X	X	
016	**Desert-dust_AS** (mmr of DU in accumulation soluble mode)	X	X	X
017	**Desert-dust_CS** (mmr of DU in coarse soluble mode)	X	X	X
018	**Desert-dust_AI** (mmr of DU in accumulation insoluble mode)	X	X	X
019	**Desert-dust_CI** (mmr of DU in coarse insoluble mode)	X	X	X
020	**NumbCon_NuS** (nmr of particles in nucleation soluble mode)	X	X	X
021	**NumbCon_AiI** (nmr of particles in Aitken insoluble mode)	X	X	X
022	**NumbCon_AiS** (nmr of particles in Aitken soluble mode)	X	X	X
023	**NumbCon_AcI** (nmr of particles in accumulation soluble mode)	X	X	X
024	**NumbCon_AcS** (nmr of particles in accumulation in soluble mode)	X	X	X
025	**NumbCon_CoI** (nmr of particles in nucleation soluble mode)	X	X	X
026	**NumbCon_CoS** (nmr of particles in nucleation soluble mode)	X	X	X
027	**Precur_DMS** (mmr of gas phase DMS from IFS-GLOMAP)	X		
028	**Precur_SO2** (mmr of gas phase SO2 from IFS-GLOMAP)	X		
029	**Precur_SO4** (mmr of gas phase H2SO4 from IFS-GLOMAP)	X	X	X
030	**Precur_Mon** (mmr of gas phase lumped monoterpene)	X	X	X
031	**Precur_SecOr** (mmr of gas phase condensable organic)	X	X	X
032	**WatVap_Md1** (mmr of water in nucleation soluble mode)	(X)	(X)	(X)
033	**WatVap_Md2** (mmr of water in Aitken soluble mode)	(X)	(X)	(X)
034	**WatVap_Md3** (mmr of water in accumulation soluble mode)	(X)	(X)	(X)
035	**WatVap_Md4** (mmr of water in coarse soluble mode)	(X)	(X)	(X)
036	**Ammonium_NS** (mmr of ammonium in nucleation soluble mode)			X
037	**Ammonium_KS** (mmr of ammonium in nucleation soluble mode)			X
038	**Ammonium_AS** (mmr of ammonium in nucleation soluble mode)			X
039	**Ammonium_CS** (mmr of ammonium in nucleation soluble mode)			X
040	**Nitrate_NS** (mmr of nitrate in nucleation soluble mode)			X
041	**Nitrate_KS** (mmr of nitrate in Aitken soluble mode)			X
042	**Nitrate_AS** (mmr of nitrate in accumulation soluble mode)			X
043	**Nitrate_CS** (mmr of nitrate in coarse soluble mode)			X
044	**Chloride_AS** (mmr of chloride in accumulation soluble mode)			X
045	**Chloride_CS** (mmr of chloride in coarse soluble mode)			X
046	**Sodium_AS** (mmr of sodium in accumulation soluble mode)			X
047	**Sodium_CS** (mmr of sodium in coarse soluble mode)			X

Table 1. List of grib items covering both the standard and nitrate-extended GLOMAP in IFS
Water content mass mixing ratios are in parentheses because they do not need to be transported.

Table 1 lists the full set of GLOMAP grib codes in the IFS required to cover both the standard and nitrate-extended configurations. The left-hand column gives the grib item number in section 212 whilst the X's in the columns on the right hand side indicate which tracers are selected for the three different configurations: a) stand-alone IFS-GLOMAP (31 transported tracers), b) standard aerosol-chemistry C-IFS-GLOMAP (29 transported tracers with the SO2 gas-phase and aqueous phase oxidation fluxes provided by the TM5 chemistry module within C-IFS) , c) nitrate-extended C-IFS-GLOMAP (39 transported tracers with NH3, HNO3 mmr's plust the SO2 oxidation fluxes provided by the TM5 chemistry module within C-IFS).

During the visit to ECMWF, the grid item numbers in Table 1 were agreed. The visit also involved considering the extra required inputs for RADAER (and it's adjoint and tangent-linear versions required for the AOD data assimilation). The group considered a document produced by Colin Johnson at the UK Met Office (appended to this deliverable report) which lists the full set of inputs required by RADAER and the name of the corresponding variable in the GLOMAP source code.

References

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Benduhn, F., Carslaw, K.S., Pringle, K., Mann, G.W., Topping, D., McFiggans, G. et al: (2014) A Computationally Efficient Hybrid Solver of Inorganic Dissolution for Use in Global Models: I. Description, Validation and First Results., in prep., for submission to *Geosci. Mod. Dev,*

Mann, G. W., Carslaw, K. S., Spracklen, D. V., et al. (2010). Description and evaluation of GLOMAP-mode: a modal global aerosol microphysics model for the UKCA composition-climate model. *Geosci. Mod. Dev.,* 3, pp. 519-551.

Morcrette, J.-J,, Boucher, O., Jones, L. et al. (2009) Aerosol analysis and forecast in the European Centre for Medium-Range Weather Forecasts Integrated Forecast System: Forward modelling, *J. Geophys. Res.,* VOL. 114, D06206, doi:10.1029/2008JD011235.

Fields Required by RADAER for Optical Depth

Colin Johnson
November 2014

Introduction

RADAER imports both prognostic and diagnostic fields in order to calculate optical depth. The prognostic fields are aerosol mass mixing ratio and number concentration. The diagnostics used are dry and wet modal diameters, density, and component partial volumes. As an upgrade to the current communication mechanism (which relies on specifying diagnostic fields in section 38), it is proposed (ticket #5049) to add these fields to section 34, and introduce a mechanism such that these are loaded automatically. Proposed upgrades to GLOMAP-mode include the ammonium nitrate scheme and the modal dust scheme, so space will be required for fields associated with these schemes.

Current Specifications

RADAER specifies the STASH numbers it requires in routine: UKCA_RADAER_INIT , and these fields should match the STASHmaster_A file. Table 1. shows the diagnostic fields currently specified in STASHmaster_A in section 38, which are derived from arrays in routine UKCA_AERO_CTL.

Array and description	STASH	MODE	Component	Used
Dry diameter (drydp)	401	nuc-sol	-	Y
	402	Ait-sol	-	Y
	403	acc-sol	-	Y
	404	cor-sol	-	Y
	405	Ait-ins	-	Y
	406	acc-ins	-	N
	407	cor-ins	-	N
Wet diameter (wetdp)	408	nuc-sol	-	Y
	409	Ait-sol	-	Y
	410	acc-sol	-	Y
	411	cor-sol	-	Y
Particle density (rhopar)	430	nuc-sol	-	Y
	431	Ait-sol	-	Y
	432	acc-sol	-	Y
	433	cor-sol	-	Y
	434	Ait-ins	-	Y
	435	acc-ins	-	N
	436	cor-ins	-	N
Partial volume (pvol, pvol_wat))	442	nuc-sol	SO4	Y
	443	nuc-sol	OC1	Y
	444	nuc-sol	OC2	N
	445	nuc-sol	H2O	Y
	446	Ait-sol	SO4	Y
	447	Ait-sol	BC	Y
	448	Ait-sol	OC1	Y
	449	Ait-sol	OC2	N
	450	Ait-sol	H2O	Y
	451	acc-sol	SO4	Y
	452	acc-sol	BC	Y
	453	acc-sol	OC1	Y
	454	acc-sol	SS	Y
	455	acc-sol	DU	N
	456	acc-sol	OC2	N
	457	acc-sol	H2O	Y
	458	cor-sol	SO4	Y
	459	cor-sol	BC	Y

Partial volume (pvol, pvol_wat)	460	cor-sol	OC1	Y
	461	cor-sol	SS	Y
	462	cor-sol	DU	N
	463	cor-sol	OC2	N
	464	cor-sol	H2O	Y
	465	Ait-ins	BC	Y
	466	Ait-ins	OC1	Y
	467	acc-ins	DU	N
	468	cor-ins	DU	N

Table 1: Description and STASH numbering for diagnostic fields used by RADAER. The comonents are: SO4 - sulphate; SS - sea-salt; OC1 - organic carbon1; OC2 - organic carbon2; BC - black carbon; DU - mineral dust; and H2O - water. The last column indicates the fields used in the five mode, four component configuration which is currently in use.

Future Requirements

In the future, it is anticipated that ammonium nitrate and modal dust will be added to GLOMAP-mode. For ammonium nitrate, the component list will be increased by the addition of nitrate (NO3), ammonium (NH4), chlorine (Cl), and sodium (Na). These components will be added to the soluble modes, NO3 and NH4 to all soluble modes, and Na and Cl only to accumulation and coarse modes.

MACC-III Deliverable D62.4

Test and evaluation of the "stand-alone" and "coupled to C-IFS" configurations of IFS-GLOMAP, the latter also with nitrate-extended GLOMAP

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Monitoring atmospheric composition & climate – III

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Work-package	Title
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Title	Test and evaluation of the "stand-alone" and "coupled to C-IFS" configurations of IFS-GLOMAP, the latter also with nitrate-extended GLOMAP
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Authors	Graham Mann, Sandip Dhomse (Leeds, U.K.) Johannes Flemming, Richard Engelen (ECMWF) Francois Benduhn (Potsdam University, Germany)
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[In case the deliverable is not a report: provide a description of it inside this box.]

Executive Summary / Abstract

This brief report describes activities carried out in MACC-III towards further development of the GLOMAP aerosol microphysics scheme in the IFS to couple to the TM5 tropospheric chemistry scheme in C-IFS.

Within MACC-II, the TM5 interface routine in C-IFS was updated to return simulated SO2 oxidation fluxes, and to pass this in to the GLOMAP interface enabling a new sulphate-coupled configuration of IFS-GLOMAP.

MACC-II Deliverable report D62.5 described preliminary work carried out at 38R2 to prepare this new "C-IFS-GLOMAP" coupled aerosol-chemistry system. Also described in the report was the plan to extend the C-IFS-GLOMAP system to also couple TM5 simulated ammonia and nitric acid to a new "nitrate-extended" version of GLOMAP, the partitioning to the particle phase then occurring to the GLOMAP size-resolved ammonium (NH_4) and nitrate (NO_3) aerosol tracers, rather than to the single-tracer NO_3 and NH_4 aerosol in C-IFS.

In most continental regions, the chemical production of nitrate aerosol tends to be limited by the availability of ammonia, with particle phase nitric acid only forming the stable ammonium nitrate species when there is excess ammonia above that required to neutralise the stronger sulphuric acid. Consequently, in order to adequately capture seasonal variations in nitrate aerosol, it is essential to also capture seasonal variations in sulphate. We therefore include in this report an assessment of IFS-GLOMAP simulated sulphate.

Section 2 presents an updated status of IFS-GLOMAP at CY40R3 with an evaluation of the simulated global distribution of sulphate, black carbon, particulate organic matter, sea-salt and dust. Section 3 shows a systematic wintertime sulphate high bias over Northern Europe in the "stand-alone" configuration of IFS-GLOMAP, with section 4 re-examining this biase in first integrations with sulphate-coupled C-IFS-GLOMAP.

Finally, in section 5 we describe work carried out towards the nitrate-extended C-IFS-GLOMAP system with test runs confirming the successful implementation of the extra aerosol tracers required for the nitrate-extension to GLOMAP. The additional FORTRAN subroutines required for nitrate-extended GLOMAP have also been added to a perforce branch in the IFS and compiled successfully.

Table of Contents

1. Introduction

During the 1st phase of MACC, the GLOMAP-mode aerosol microphysics scheme (Mann et al., 2010, 2012) was incorporated into the IFS to upgrade the single-moment aerosol scheme implemented in GEMS (Morcrette et al., 2009), providing information on aerosol size and number for improved representation of aerosol-radiation and aerosol-cloud interactions. As part of MACC-II, the RADAER module (Bellouin et al., 2011) was added to the CY38R1 implementation of IFS-GLOMAP, to diagnose aerosol optical properties for each of the size modes, accounting for the simulated internally-mixed composition and size.

Within MACC-II, the IFS-GLOMAP interfaces were adapted (at CY38R2) in preparation for a fully integrated aerosol-chemistry configuration of IFS-GLOMAP with coupling to gas phase and aqueous phase SO2 oxidation calculated within the TM5 chemistry scheme within C-IFS.

MACC-III deliverable report D62.1 described work carried out at CY40R3 to prepare for the upgrade of this chemistry-aerosol C-IFS-GLOMAP system to use a new "nitrate-extended" version of GLOMAP (Benduhn et al., 2015).

Accurately characterising the seasonal cycle of nitrate aerosol requires also for the sulphate seasonal cycle to be well represented, since biases in sulphate affect the amount of free ammonia available to form ammonium nitrate.

The first part of this deliverable report (section 2) therefore presents an evaluation of the sulphate concentrations simulated in IFS-GLOMAP, comparing to surface observations in Europe, North America and the North Atlantic.

The 2nd part of this deliverable report (section 3) repeats these model-measurement comparisons based on first integrations with the "sulphate-coupled" C-IFS-GLOMAP system. In particular we show that the coupling to the TM5 sulphur chemistry makes an important improvement to the simulation of wintertime sulphate in northern Europe.

Section 4 of this report describes work to carry out the implementation of the required additional tracers to IFS-GLOMAP with test runs using the existing GLOMAP code confirming this preliminary configuration. A perforce branch containing the nitrate-extended GLOMAP routines has been added to the IFS and these new routines have successfully compiled.

2. Evaluation of speciated aerosol mass in IFS-GLOMAP

We begin the report with a section by presenting results which constitute a major milestone for IFS-GLOMAP, achieved early in MACC-III, but not yet reported in a deliverable report

An ongoing problem with IFS-GLOMAP at CY38R1 was that the simulation of mineral dust was being corrupted (see section 3 of MACC-II Deliverable Report D62.5). Following work by Richard Engelen to port the IFS-GLOMAP codebase to CY40R1 early in MACC-III the suspected diagnosis reported in the D62.5 report was confirmed as being caused by the over-write of the GLOMAP dust tracers duing re-initialisation at the start of forecast cycles.

Figures 1, 2 and 3 present evaluation of simulated speciated aerosol properties against surface observations from monitoring sites in Europe (EMEP), N. America (IMPROVE) and for marine sites (the University of Miami network of monitoring sites).

The observational datasets used and evaluations carried out are a repeat of those presented in the GLOMAP-mode description and evaluation paper (Mann et al., 2010), but applied to the reference CY40R3 IFS-GLOMAP run.

This simulations were forecast-cycling experiments at T255L60 resolution without any AOD data assimilation, and are analogous to the simulations with the mass-based scheme as presented in Morcrette et al. (2009).

Whereas other partners in MACC-III are evaluating the aerosol optical properties of the overall multi-component aerosol, here we compliment those evaluations by assessing the global disitrbution of each aerosol component simulated in themodel covering sulphate, black carbon (BC), particulate organic matter (POM), sea-salt and dust.

The comparisons in Figures 1 to 3 represent a first-order assessment of the annual-mean global surface distribution to illustrate the current status of the model. The sulphate, BC and POM observations are from the year 2000, whereas this particular s simulation (b1e3) is running with online re-analysis meteorology for the year 2008.

A more detailed assessment of the IFS-GLOMAP simulated aerosol properties is being carried out for CY40R3 runs and will be written up as part of the IFS-GLOMAP description and evaluation paper current in preparation (Woodhouse et al., 2015) which compares results of year-2003 forecast-cycling experiment against observational datasets specific for that particular year.

Figures 1 and 2 illustrate that the model is representing the surface global distribution of sulphate, BC and POM in good agreement with the observations. Figure 3 illustrates that the sea-salt and dust aspects in IFS-GLOMAP are operating qualitatively quite well with the dust having reasonably good correlation (R=0.67) against the observations. However, whereas the sulphate, BC and POM (which are all in the fine mode) were all also in good quantitative agreement with the observations, there is a substantial low bias apparent in the IFS-GLOMAP simulation of the sea-salt and dust in these initial 40R3 simulations.

3. Assessment of IFS-GLOMAP sulphate in "stand-alone" configuration

In section 2, we gave an overview of the current implementation of the IFS-GLOMAP system at the latest cycle (40R3). The comparisons suggested that simulated surface sulphate in the model was in good agreement with the observations on the annual mean. Those runs were using the "stand-alone" configuration of IFS-GLOMAP whereby sulphate production proceeds following the latitudinally-varying timescale approach described in Morcrette et al. (2009) and used in the MACC re-analysis (Innes et al., 2013).

Previous evaluation of the seasonal cycle of sulphate at CY38R1 has shown that although the simplified sulphate production approach generally agrees quite well with sulphate observations on an annual mean basis, when one considers the seasonal cycle of sulphate clear biases are apparent. For example we found that simulated sulphate concentrations in Northern Europe were substantially high biased during wintertime.

Figure 4 assesses simulated wintertime sulphate across Europe in the latest cycle (40R3), considering the February-mean of the 2008 stand-alone IFS-GLOMAP run (b1fv). It is apparent that the high sulphate bias in Northern Europe encountered in stand-alone IFS-GLOMAP at 38R1 is also apparent at 40R3, suggesting this is a systematic bias in the model.

In the next section we use this February sulphate comparisons to year-2000 EMEP sites as a test case to assess the benefit of coupling the sulphate production in TM5 to GLOMAP.

4. Improvement of IFS-GLOMAP sulphate with coupling to TM5 chemistry

Figure 5 presents the first results from the sulphate-coupled C-IFS-GLOMAP aerosol system with the gas phase and aqueous phase SO2 oxidation fluxes from TM5 being passed to GLOMAP to drive the sulphate production in the aerosol microphysical module. The model has so far only been run for a few months, which is why the February 2008 monthly-mean was chosen, allowing for 2 months spin-up from the start date of 1st December 2007.

Although Figure 5 is only preliminary, the assessment shows promising results with respect to the wintertime sulphate high bias in Northern Europe identified in section 3. The model is in good agreement with observations in that region (Figure 5b), although in Southern Europe the model is low biased against the measurements at this time of year.

Considering the Eastern US, sulphate-coupled C-IFS-GLOMAP is now low biased against the measurements in February (Figure 5c), whereas the stand-alone IFS-GLOMAP was in good agreement (Figure 4c).

In marine regions, the simulated sulphate concentrations are much lower than in stand-alone IFS-GLOMAP, and much lower than the climatological University of Miami observations for that month. One should note that these marine observations were averaged over the 1990s so since anthropogenic SO2 emissions have dropped substantially since then, so the model (run with year-2000 anthropogenic emissions) might be expected to have some inherent high bias there, particularly during winter when DMS concentrations will be very low..

Although these initial set of comparisons suggest the sulphate-coupled C-IFS-GLOMAP system is performing worse against the measurements, it is worth re-iterating that these results are only preliminary.

The benchmark observations we have assembled have already proved very useful for 1st order assessment of each aerosol tupe (sulphate, sea-salt, BC, POM and dust). We identified already seasonal and regional biases to be improved in ongoing development and tuning.

5. Implementation of nitrate-extended GLOMAP into the IFS

The first MACC-III Deliverable report D26.1 describes the changes required to the IFS-GLOMAP system to implement the nitrate-extended version of GLOMAP into the IFS. The initial task identified there was to update the namelists for IFS-GLOMAP adding the required extra 10 tracers for the size-resolved ammonium (+4) and nitrate (+4) and replacing the existing two sea-salt tracers (-2) with separate sodium (+2) and chloride (+2) tracers in the accumulation and coarse soluble modes.

Since that first deliverable report we have now implemented those changes following exactly the grid item numbers described in Table 1 of that report. We have successfully carried out a test run which uses the standard IFS-GLOMAP code-base in sulphate-coupled C-IFS-GLOMAP configuration, but additionally has the extra 10 tracers running (with zero values). We have established that that initial run gives equivalent results.

The 2nd milestone reached since the D26.1 report is that the 18 new subroutines which together constitute the "dissolution solver" for GLOMAP (as described in Benduhn etal., 2015) have now been added to a perforce branch. The names of the 18 new routines are listed below for reference. In addition to those new routines, 6 existing GLOMAP routines were updated to interface with the new module and these are also listed below. Finally the interface routines UKCA_MODE_EMS_IFS and UKCA_AERO_STEP_IFS were updated to provide the required switches and extra input/output variables to GLOMAP but with the main switches IDISS_ON and IDIFF_ON set to zero which essentially switches off the dissolution module with the nitrate-extended codebase then operating in the same way as in the old codebase.

A repeat run of the 10-extra-tracer configuration of sulphate-coupled C-IFS-GLOMAP, using the updated branch has been submitted and the new routines compile.

New routines:
1) ukca_mode_chemistry_solver.F90
2) ukca_mode_transport_solver.F90
3) ukca_mode_diss_combsolv.F90
4) ukca_dissolution.F90
5) ukca_mode_drydensity.F90
6) ukca_mode_imode_density.F90
7) ukca_mode_density.F90
8) ukca_prim_ss_wet.F90
9) ukca_mode_ionorgsetup.F90
10) ukca_mode_lisnan.F90
11) ukca_mode_chosencubic.F90
12) ukca_mode_cubicroot.F90
13) ukca_mode_quarticroot.F90
14) ukca_mode_quadbiden.F90
15) ukca_mode_hexbiden.F90
16) ukca_mode_sulfbiden.F90
17) ukca_mode_ionbalance_check.F90
18) ukca_mode_int_ssflux.F90

Finally we note that the main paper describing the nitrate-extended GLOMAP (Benduhn et al., 2015) has, in the first half of 2015 been substantially revised and improved and a final draft is currently with all co-authors, with submission to Geoscientific Model Development planned for the end of July 2015. The paper describes the "dissolution module" in detail, evaluating its performance in box model simulations, assessing the size-resolved partitioning of ammonia and nitric acid over a range of conditions, and comparing the hybrid scheme against more conventional equilibrium partitioning approaches.

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Benduhn, F. et al. (2015) A Computationally Efficient Hybrid Solver of Inorganic Dissolution for Global Models: I. Description, Validation & First Results., to be submitted to Geosci. Mod. Dev.

Innes, A. et al. (2013), The MACC reanalysis: an 8 yr data set of atmospheric composition, *Atmos. Chem. Phys.*, 13, 4073–4109.

Mann, G. W. et al. (2010) Description and evaluation of GLOMAP-mode: a modal global aerosol microphysics model for the UKCA model, *Geosci. Model Dev.*, 3, 519–551.

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Morcrette, J.-J. et al. (2009) Aerosol analysis and forecast in the ECMWF Integrated Forecast System: Forward modeling, J. Geophys. Res., vol. 114, D06206, doi:10.1029/2008JD011235

Fig. 1: Annual mean sulphate simulated in stand-alone IFS-GLOMAP (b1e3)
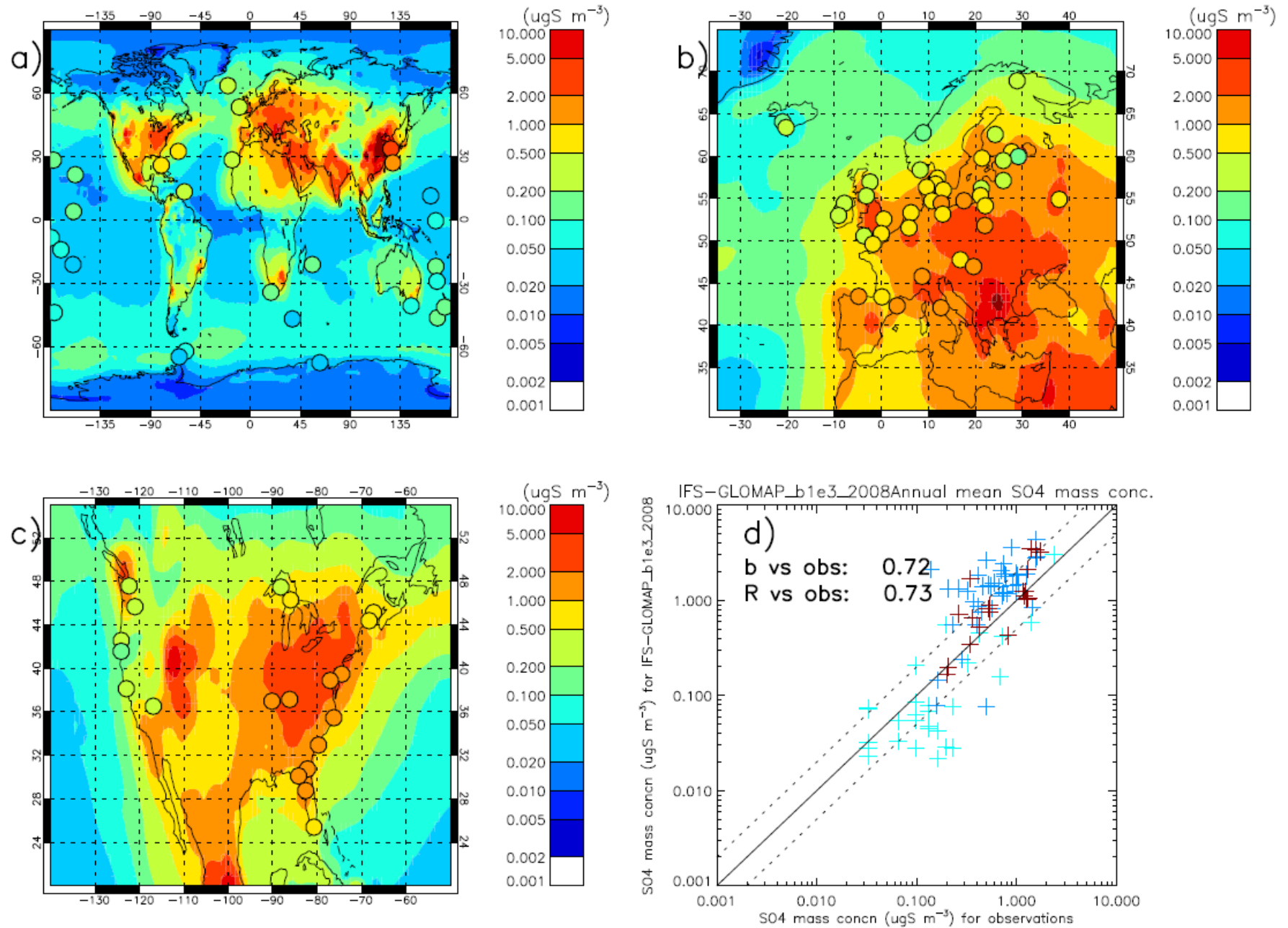
Fig. 2: Annual mean EC & POM simulated in stand-alone IFS-GLOMAP (b1e3)
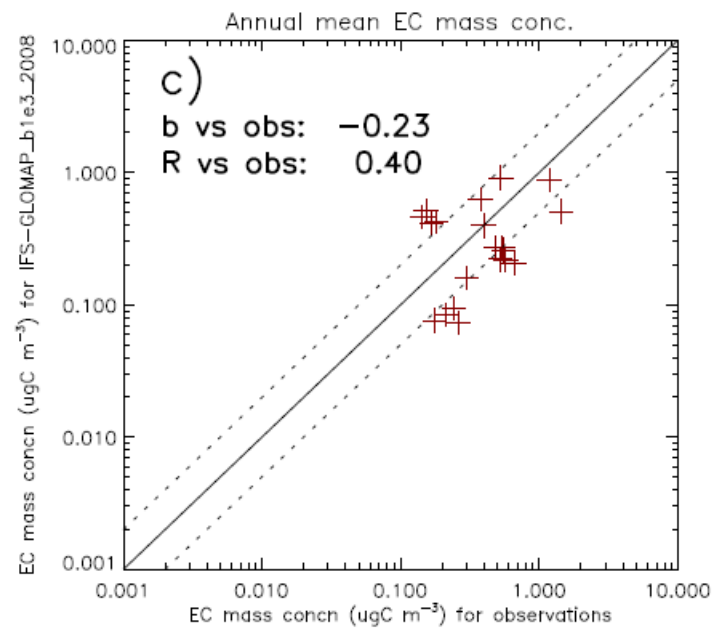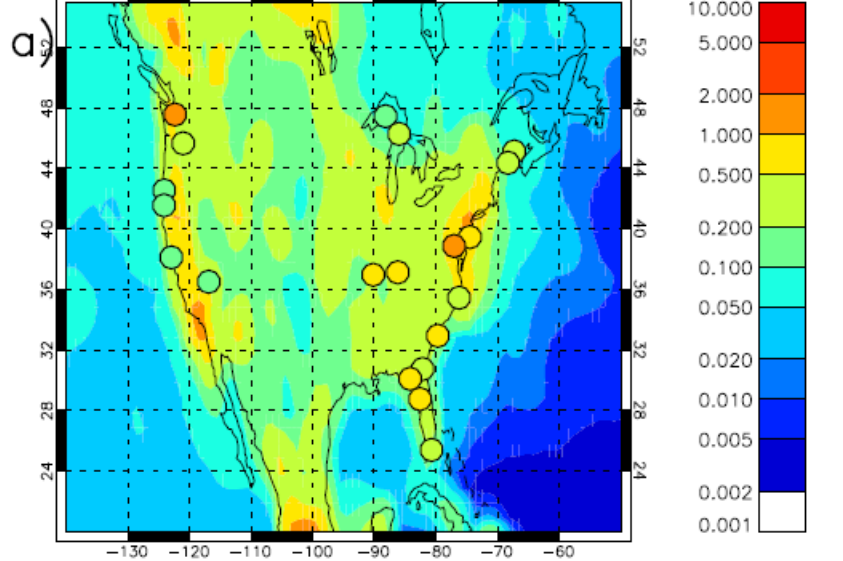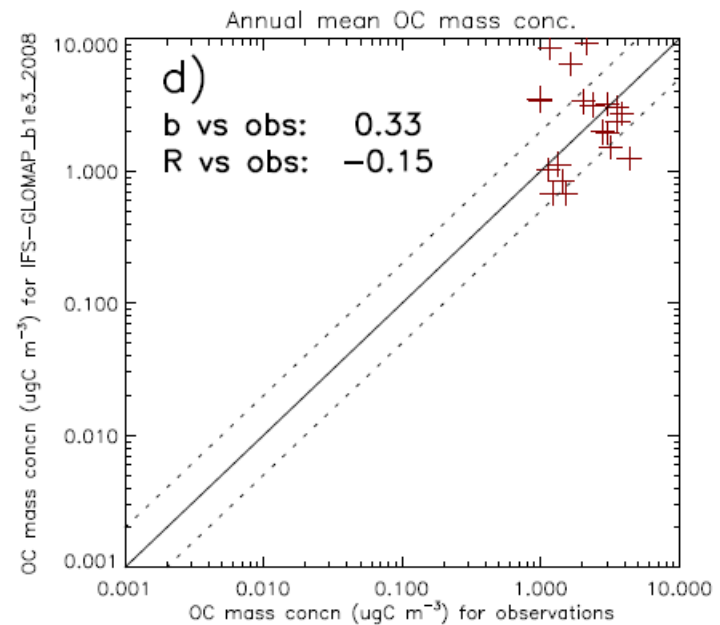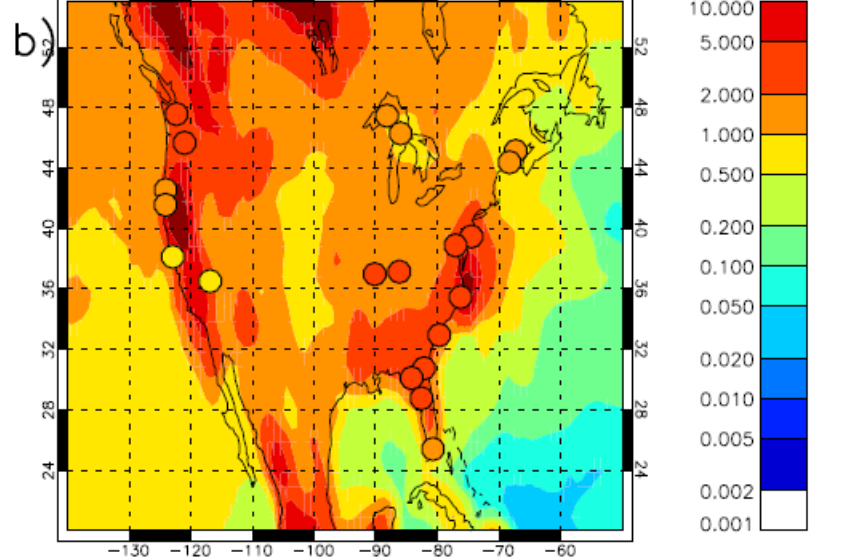
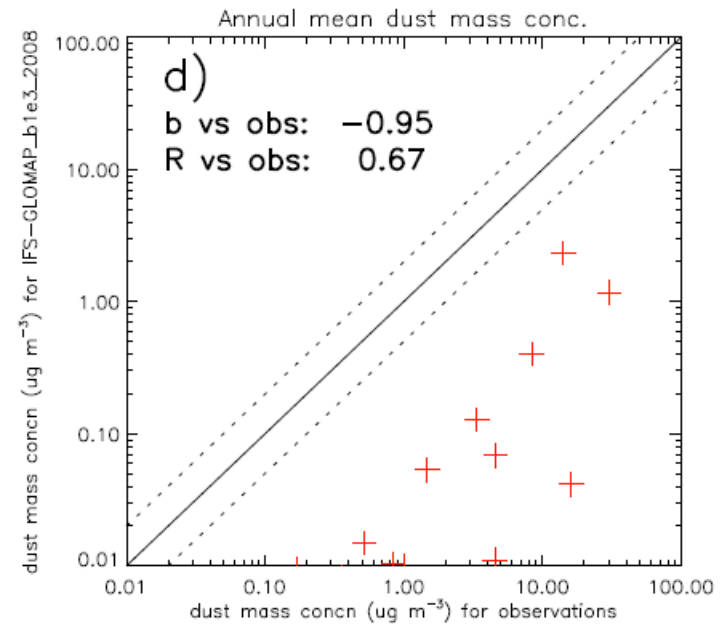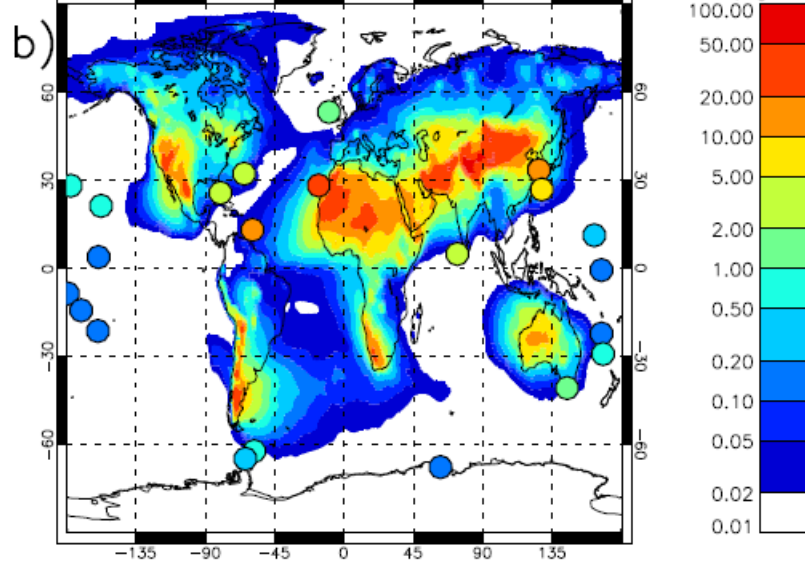# Fig. 3: Annual mean NaCl, DU simulated in stand-alone IFS-GLOMAP (b1e3)
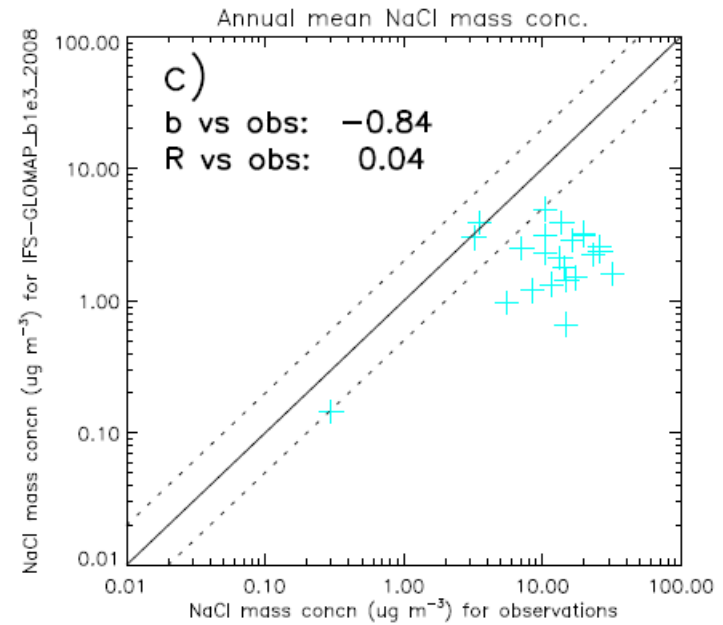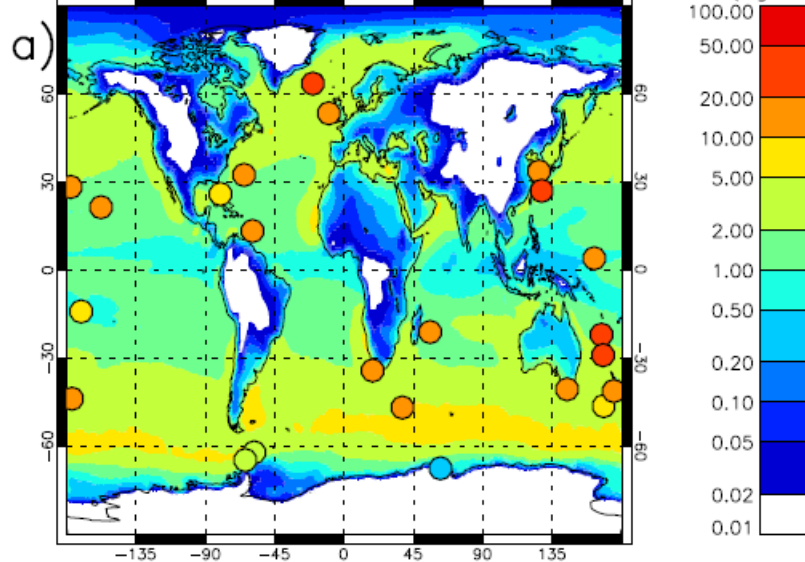
Fig. 4: February-mean sulphate simulated in stand-alone IFS-GLOMAP (b1fv)
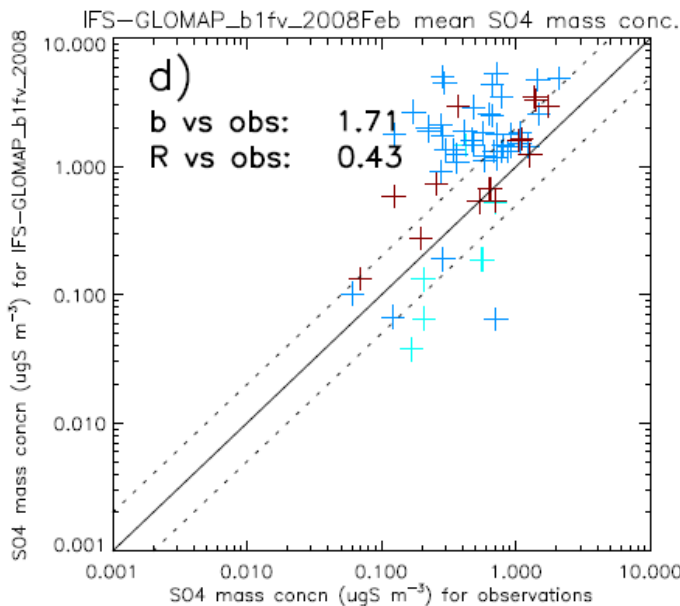
Fig. 5: February-mean sulphate simulated in sulphate-coupled C-IFS-GLOMAP (b1ft)
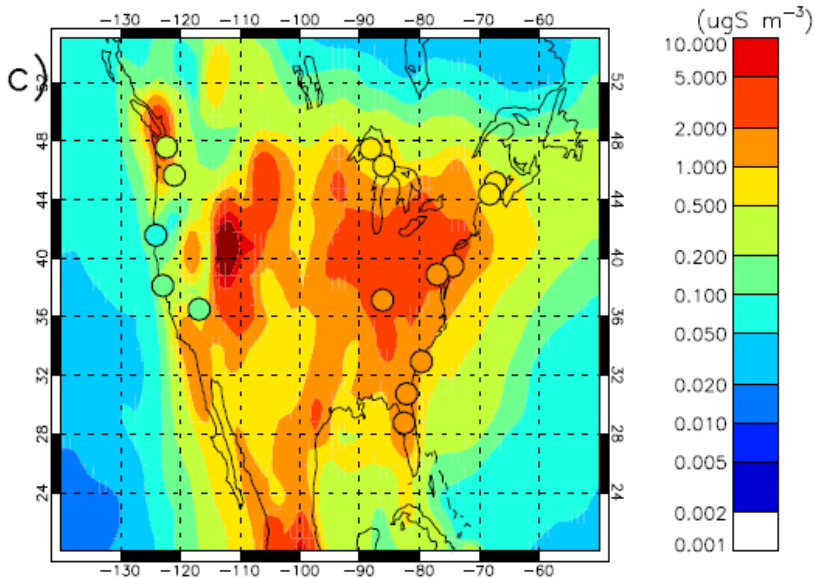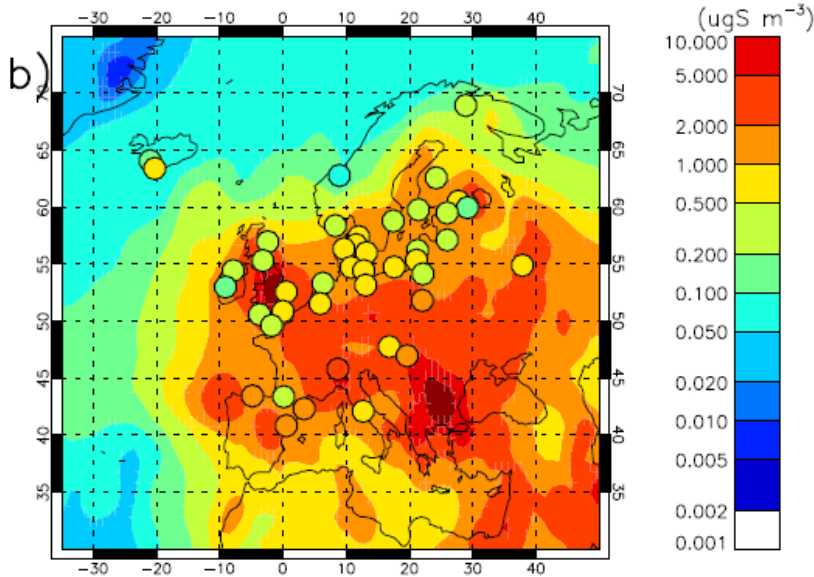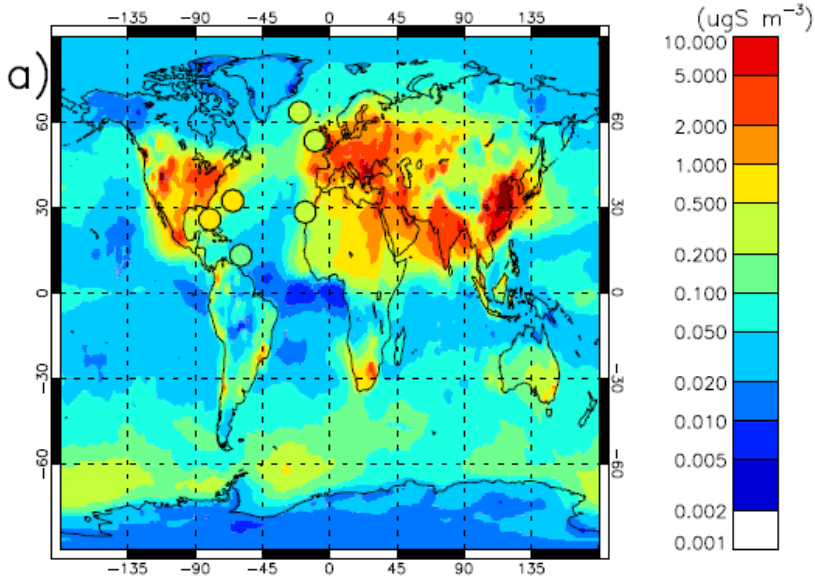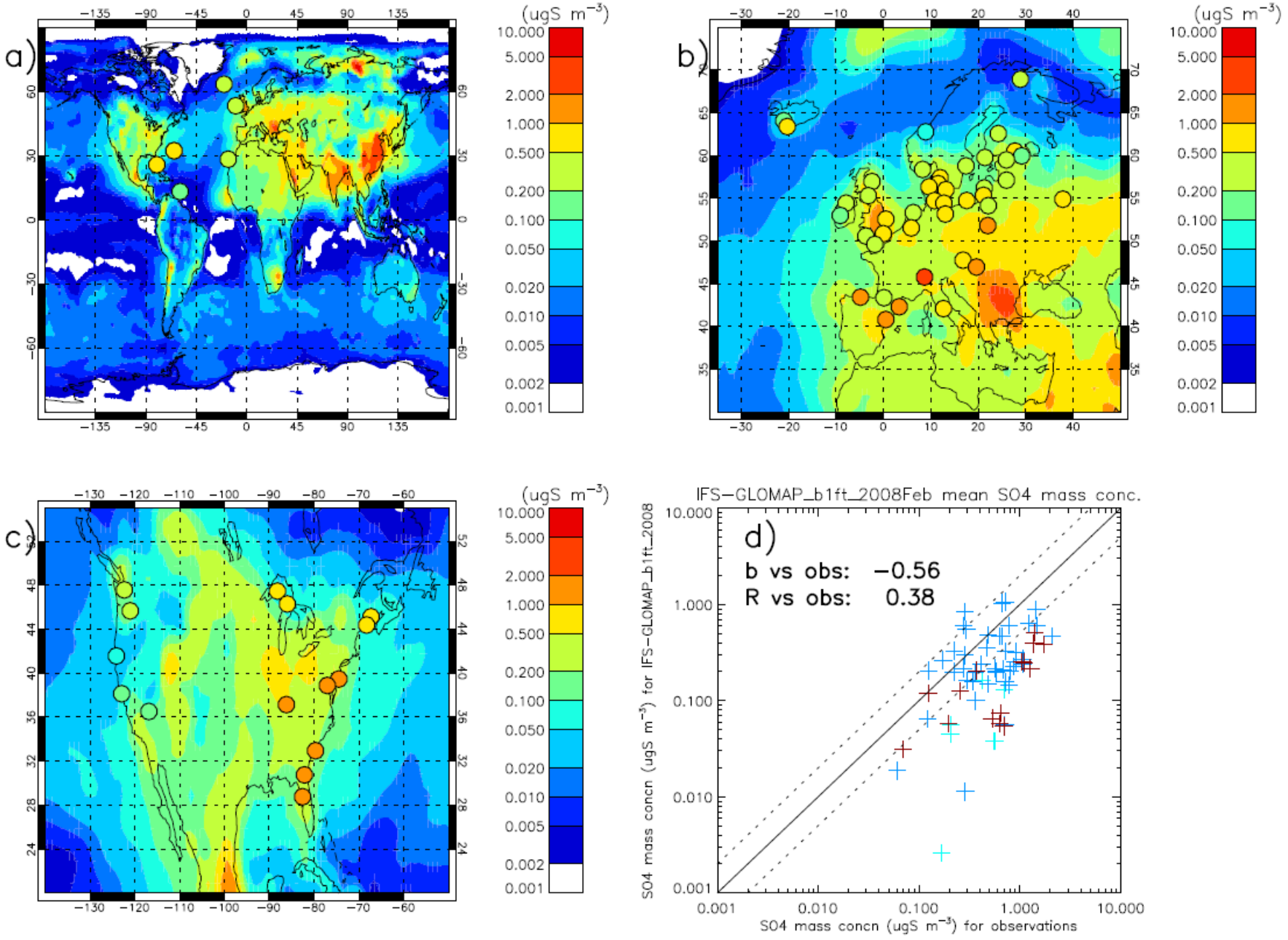
Comparison of vertical profile and surface extinction coefficient against observations.

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Work-package	Title
Deliverable	D65.3
Title	Comparison of vertical profile and surface extinction coefficient against observations
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Authors	Graham Mann (University of Leeds, U.K.)
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[In case the deliverable is not a report: provide a description of it inside this box.]

Executive Summary / Abstract

This brief report describes activities carried out during MACC-III to adapt the IFS-GLOMAP aerosol optical properties module "RADAER" to additionally return 3D backscatter at selected wavelengths and additionally convert that into attenuated backscatter profiles for direct comparisons to space-borne or ground-based lidar measurements.

We refer to this capability as a "lidar emulator" as it derives from the model the quantity measured by the lidar (attenuated backscatter) rather than comparing extinction which requires an assumption for an aerosol type dependent extinction-to-backscatter ratio.

This report presents results from research carried out principally by Stuart Young and Martin Cope at CSIRO, Aspendale, Australia. Rather than provide a conventional report, we instead have chosen to present the deliverable in the form of an extended abstract produced by Dr. Young for the 27th International Laser Radar Conference in New York, USA (July 2015).

The research forms part of an collaboration between the University of Leeds and CSIRO on aerosol modelling with the GLOMAP aerosol microphysics scheme. The CSIRO air quality modelling team have implemented GLOMAP into their high-resolution chemistry transport model TAPM and the CSIRO climate modelling team use GLOMAP as implemented within the UM-UKCA composition-climate model via the ACCESS partnership with the UK Met Office.

As part of a visiting scientist fellowship funded by the UK National Centre for Atmosphere Science and a CSIRO Frolich fellowship, he University of Leeds MACC-III PI Graham Mann visited CSIRO Aspendale over 6 weeks during July and August 2014 where the research was discussed with Dr. Cope & Dr. Young.

The extended abstract presented here includes a case study to compare a transect of 532nm total attenuated backscatter derived from TAPM-GLOMAP over Australia against a CALIPSO overpass during October 2006.

The lidar emulator produced model attenuated backscatter profiles retain the full information on size-resolved aerosol composition as simulated by GLOMAP and is a potentially powerful technique by which C-IFS with GLOMAP could provide an observational operator for satellite-borne lidar such as CALIPSO.

SIMULATION OF CLOUD-AEROSOL LIDAR WITH ORTHOGONAL POLARIZATION (CALIOP) ATTENUATED BACKSCATTER PROFILES USING THE GLOBAL MODEL OF AEROSOL PROCESSES (GLOMAP)

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ABSTRACT

To permit the calculation of the radiative effects of atmospheric aerosols, we have linked our aerosol-chemical transport model (CTM-GLOMAP) to a new radiation module (UKCA-RADAER). In order to help assess and improve the accuracy of the radiation code, in particular the height dependence of the predicted scattering, we have developed a module that simulates attenuated backscatter (ABS) profiles that would be measured by the satellite-borne Cloud-Aerosol Lidar with Orthogonal Polarization (CALIOP) if it were to sample an atmosphere with the same aerosol loading as predicted by the CTM. Initial results of our comparisons of the predicted ABS profiles with actual CALIOP data are encouraging but some differences are noted, particularly in marine boundary layers where the scattering is currently under-predicted and in dust layers where it is often over-predicted. The sources of these differences are being investigated.

1. INTRODUCTION

Atmospheric aerosol is well known to lead to perturbations in the radiation balance, via direct, and indirect (i.e. changes to cloud properties) effects. Accurate representation of the aerosol size distribution and characteristics such as solubility are essential if models are to simulate correctly the coupling between aerosol loading and radiative forcing.

Because the vertical distribution of aerosol layers in the atmosphere, in addition to their optical properties, can have a significant effect on their radiative impact, we consider it necessary to assess the accuracy of our model's predictions of those vertical profiles. As we apply our model over scales ranging from continental to global, we need to compare with vertically resolved measurements made on such scales. An ideal source of such data is the CALIOP lidar on board the CALIPSO satellite [1]. While it is common to compare model predictions with measurements of such quantities as aerosol optical depth or particulate extinction coefficient, it should be remembered that CALIOP is an elastic-backscatter lidar and does not measure either of these quantities directly. Rather it retrieves these quantities from its primary measurement, the attenuated backscatter coefficient, via a combination of analysis algorithms [1,2] and an optical model of the scattering properties of the aerosol (or cloud) particles. The optical model can only describe the average properties of an identified aerosol type. A misidentification of the aerosol type, or natural variation of the optical properties from the average values, will lead to errors, of various magnitudes, in the retrieved extinction and optical depths [3]. As a result, a difference between simulated and measured profiles of a certain optical quantity could be the consequence of an incorrect prediction of aerosol concentrations, location or type, or of optical properties on the side of the chemical transport model (CTM-GLOMAP), or of errors in the optical properties used to retrieve the profiles from the measurements. In some cases, this is effectively comparing one model with another, which is neither what is intended nor is it very informative. To overcome these problems, we choose instead to compare the fundamental lidar measured quantity, the attenuated backscatter profile, with simulated profiles derived from the radiation module (UKCA-RADAER) that is used by our CTM. Attenuated backscatter is the product of the sum of the molecular and particulate backscatter coefficients at any height and the molecular and particulate two-way transmittances between that height and the lidar. It is simply the calibrated backscattered power

measured by the lidar corrected for the range-squared decrease in signal with distance from the lidar. In this way all of the uncertainties are on one side of the comparison thus permitting unambiguous assessment of the model.

2. METHODOLOGY

(a) The Models

In our modeling system, continental-scale atmospheric transport is modeled using a coupled system that comprises (1) the CSIRO Conformal-Cubic Atmospheric Model [4,5] for simulating weather, (2) a population-based anthropogenic emission inventory with natural primary emission sources such as sea salt, wind-blown dust, plus biogenic and fire emissions, and (3) a chemical transport model (CTM,[6]) for simulating the atmospheric chemical transport and subsequent fate, via wet and dry deposition, of gaseous and particulate species. It has a comprehensive chemistry incorporating the Carbon Bond 5 mechanism [7], the Volatility Basis Set approach [8] for secondary organic aerosols, and the ISORROPIA-II model [9] for secondary inorganic aerosol modeling.

The CTM is coupled with the GLObal Model of Aerosol Processes (GLOMAP, [10]), which is a comprehensive, size-resolving global aerosol model. In this work CTM-GLOMAP employs 7 modes and 5 components. Its boundary and initial conditions for aerosol components and modes are obtained from an instance of GLOMAP running in a nudged global general circulation model. The CTM-GLOMAP domain for the Australia continent has a resolution of 0.5^{o}.

The optical properties such as aerosol optical depth (AOD), and aerosol backscatter and extinction coefficients are calculated at each model grid by the RADAER module via a Mie look-up table for the appropriate sizes and refractive indices. The lidar signals are then simulated, as described below, at each of the 19 model levels, which extend from 0.02 km to 8 km above the surface, with a vertical resolution that varies from 0.02 km near the surface to 2 km at the top of the simulation. The comparison with the measurements is then currently done off line, by extracting simulated profiles from the model output file at each model grid point along the CALIPSO ground track of interest.

(b) The Simulator

In each model grid cell, the model system predicts the aerosol components and their size modes. For each of these aerosol components, the particulate backscatter, β_P, and extinction coefficients, σ_P, are then obtained at the CALIOP wavelengths (532 nm and 1064 nm) via a pre-calculated Mie look-up table. In addition, the atmospheric temperature and pressure profiles, available from the modeled meteorology, can be used to calculate the molecular number density profile and, hence, the backscatter, β_M, and extinction coefficient, σ_M, profiles at the lidar wavelengths. The ozone number density is also available from the model allowing the ozone absorption profile, $\alpha_{O3}(z)$, to be calculated. (Ozone absorption is only significant at the shorter wavelength.) It is then a simple matter to calculate profiles of attenuated (total) backscatter:

$$\beta_T'(z) = [\beta_M(z) + \beta_P(z)]T_M^2(z_s, z)T_P^2(z_s, z),$$

where

$$T_M^2(z_s, z) = \exp\left\{-2\int_{z_s}^{z}[\sigma_M(r) + \alpha_{O_3}(r)]dr\right\},$$

and

$$T_P^2(z_s, z) = \exp\left\{-2\int_{z_s}^{z}\sigma_P(r)dr\right\}$$

are, respectively, the molecular and particulate two-way transmittance profiles. The profile of attenuated scattering ratio, $R'(z)$, is obtained from the attenuated total backscatter coefficient profile by dividing by the profile of attenuated molecular backscatter,

$$\beta_M'(z) = \beta_M(z)T_M^2(z_s, z),$$

to give

$$R'(z) = [1 + \beta_P(z)/\beta_M(z)]T_P^2(z_s, z).$$

To simulate the satellite-borne CALIOP profiles, the calculation is started at the top of the atmosphere (or the satellite altitude z_S), and proceeds down towards the surface in order to account correctly for the increasing signal attenuation with range from the satellite (decreasing height).

(c) CALIOP Attenuated Backscatter Profiles

The CALIOP data used in the comparisons here are the "Total_Attenuated_Backscatter_532" from the CALIPSO, level-1, version 3 files and the "Feature_Classification_Flags" in the corresponding, level-2, vertical feature mask (VFM) files.

Although the aim of this exercise is to compare measured and modeled profiles in an atmosphere containing air molecules and aerosol particles, in practice, the measured atmosphere often also contains clouds, which can complicate the comparison somewhat. To facilitate the comparisons, the measured data were filtered to exclude from the calculated average profiles all points in any single profile below the top of cloud layers that were identified in the corresponding VFM profiles. The filtered profiles were then averaged to produce a horizontal resolution comparable to that of the model in the domain of interest (10°S - 45°S, 110°E to 165°E). The vertical resolution of the measured data was, however, not degraded to that of the model but kept at 30 m over the complete height range.

3. RESULTS

In Figure 1 we present an example of our comparisons. The 532-nm attenuated total backscatter measured as CALIPSO passed over Australia on 7 October 2006 at approximately 1621 UTC is shown as a function of height and latitude in (a) with the simulation in (b). The aerosol subtype as identified by CALIPSO's algorithms is shown in (c). Notable features are a strongly scattering marine boundary layer extending to an altitude of 1 km to the North and 2 km to the South of the continent, and a deep moderately strongly scattering aerosol layer that extends to nearly 4 km altitude at latitudes of 20° and 30° S. Between these latitudes, the strength of the signal decreases markedly to the extent that it cannot be detected by the algorithms and does not appear in the VFM. CALIPSO's algorithms identify these aerosols as being predominantly "polluted dust" (a mixture of dust and smoke) with an indication that the weaker signal recorded between these latitudes is from pure dust.

The model generally correctly reproduces the location and heights of the marine layers, although the southern layer is slightly too low in places. The height of the continental layers is also fairly well reproduced as is the extension of the dust layer above the southern marine layer.

Although the horizontal and vertical locations of the various layers are correctly reproduced in the simulation shown, the magnitudes of the simulated signals are, in some places, rather different from what are observed.
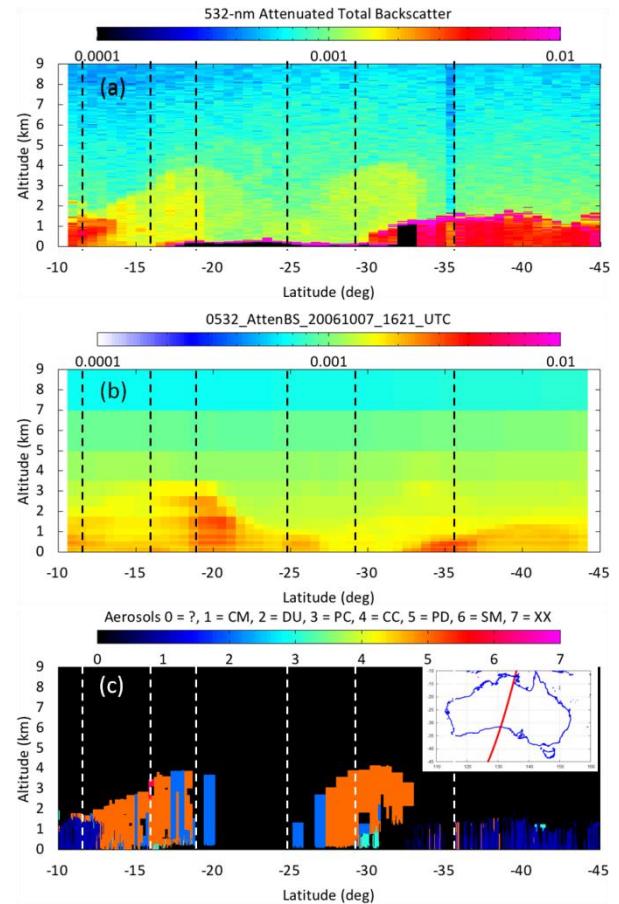

Figure 1. 532-nm Attenuated Total Backscatter (a) CALIOP, (b) Simulation. (c) Aerosol sub-type Vertical Feature Mask. CM = Clean Marine, DU = Dust, PC = Polluted Continental, CC = Clean Continental, PD = Polluted Dust, SM = Smoke, XX = not defined. Vertical, dashed lines indicate locations of profiles in Fig. 2. Inset shows CALIPSO ground track over Australia on 7 October 2006 at ~1621 UTC.

In order to study these differences in more detail, in Figure 2 we compare measured and modeled profiles of attenuated backscatter. The profiles correspond to the locations of the dashed vertical lines in Figure 1. Note that the magnitudes of the simulated profiles are larger than those of the

measured profiles in the free troposphere. This is a result of the additional atmospheric attenuation that was measured between the lidar (at 705 km) and the top of the simulation (at ~ 9km) that has not been corrected for in these figures as it helps separate the profiles horizontally and, thereby, improve legibility. In the first profile, at 11.51 ° S, this difference is increased by the attenuation caused by a layer of high cloud above 9 km and not shown here. The comparison of profiles shows the marked under-prediction of scattering in the marine layers in (a) and (f), reasonable agreement in the polluted dust in (b), but less so at (e), and a significant over-estimation of the signal from dust at (c) and (d). The extent to which these differences are attributable to incorrectly predicted number densities, hydration (for the marine layers) or optical properties (e.g. the use of Mie-scattering code for dust) is being investigated and will provide useful information for the development and improvement of our model and radiation code.
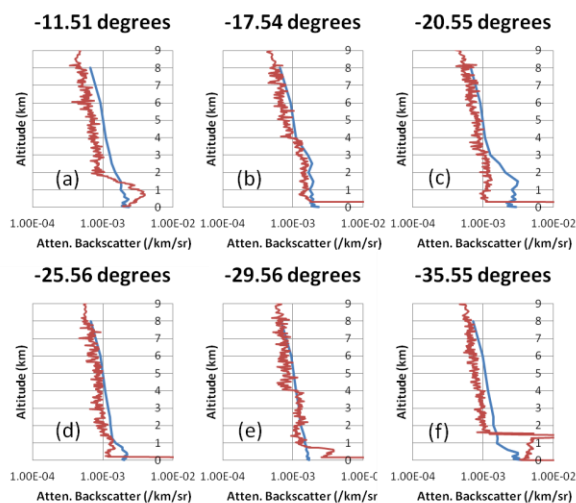

Figure 2. Profiles of 532-nm Attenuated Total Backscatter at the locations indicated by the dashed lines in Fig. 1. The red, noisy profiles are CALIOP data while the blue, smooth profiles are the simulations.

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