Introducing IFS-CB05-BASCOE-GLOMAP

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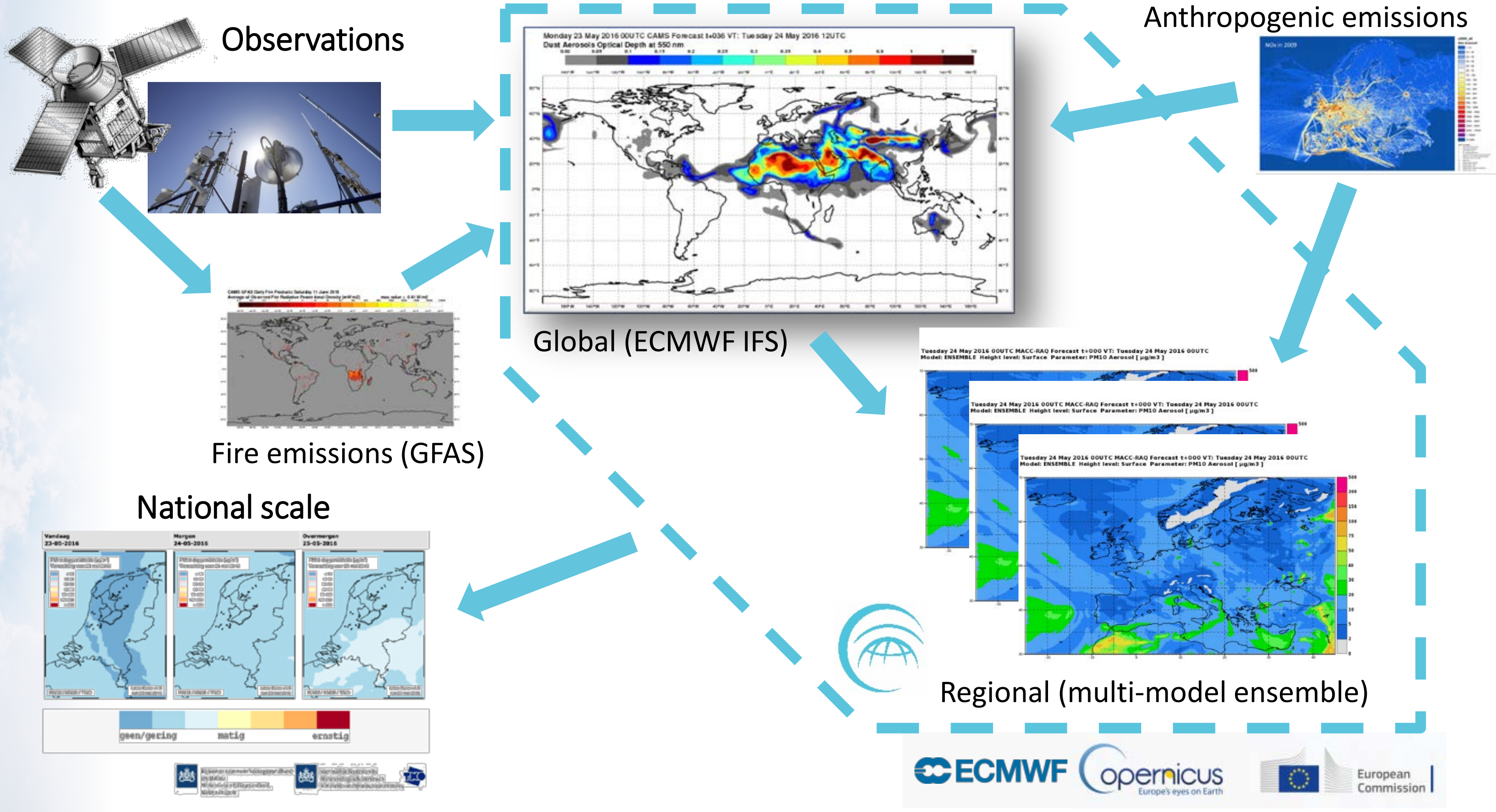
The CAMS system



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Operational CAMS global system: IFS-CB05-AER

Standard IFS dynamics and physics

(as used in ECMWF NWP but at lower resolution)

AER bulk/bin aerosol

(based on LOA/LMDZ scheme)

Reddy et al. (2005)
Morcrette et al. (2009)
Rémy et al. (2019)

CB05 tropospheric chemistry

(based on TM5 CTM;
Euler Backward Iterative solver)

Yarwood et el. (2005)
Huijnen et al. (2010)
Flemming et al. (2015)

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Extended CAMS global system: IFS-CB05-BASCOE-GLOMAP

Standard IFS dynamics and physics

(as used in ECMWF NWP but at lower resolution)

GLOMAP-mode

2-moment modal aerosol

Mann et al. (2010)

IFS implementation begun under MACC/-II

CB05-BASCOE

Huijnen et al. (2016)

CB05 tropospheric chemistry

(based on TM5 CTM)

Yarwood et al. (2005)
Huijnen et al. (2010)
Flemming et al. (2015)

BASCOE stratospheric chemistry

(based on BASCOE CTM)

Errera et al. (2008, 2019)
Chabrillat et al. (2018)

(3rd order Rosenbrock solver via KPP)

Combining tropospheric and stratospheric chemistries

Tropospheric species (CB05)

Pb	*PAR*	ACO2
C_2H_4	*OLE*	$IC_3H_7O_2$
C_2H_6	*ALD2*	$HYPROPO_2$
C_2H_5OH	*ROOH*	*ROR*
C_3H_8	PAN	*RXPAR*
C_3H_6	*ONIT*	XO_2
C_5H_8	SO_2	XO_2N
$C_{10}H_{16}$	DMS	
CH_3COCHO	MSA	
CH_3COCH_3	NH_2	
CH_3OH	NH_3	
HCOOH	C_2O_3	
MCOOH	ISPD	

SO_4
$NO_3^{(A)}$
NH_4

Pseudo-aerosol species

O_3	N_2O_5
OH	Rn
H_2O_2	
CO	
CH_2O	
CH_3O_2	
CH_3OOH	
CH_4	
NO	
NO_2	
NO_3	
HNO_3	
HO_2NO_2	

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Combining tropospheric and stratospheric chemistries

Stratospheric species (BASCOE)

O_3	N_2O_5
OH	Rn
H_2O_2	
CO	
CH_2O	
CH_3O_2	
CH_3OOH	
CH_4	
NO	
NO_2	
NO_3	
HNO_3	
HO_2NO_2	

O	HCl	CH_3Br	CFC-115
$O^{(1D)}$	HOCl	CH_2Br_2	HCFC-22
H	CH_3Cl	$CHBr_3$	HA-1301
H_2	CH_3CCl_3	$BrONO_2$	HA-1211
H_2O	CCL_4	BrO	
CH_3	$ClONO_2$	HBr	
CH_3O	$ClNO_2$	HOBr	
HCO	ClO	BrCl	
CO_2	OClO	HF	
N	ClOO	CFC-11	
N_2O	Cl_2O_2	CFC-12	
Cl	Br	CFC-113	
Cl_2	Br_2	CFC-114	

OCS
SO_3
H_2SO_4

Sulphur extensions

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Combining tropospheric and stratospheric chemistries

Tropospheric species (CB05)

Pb	*PAR*	ACO2
C_2H_4	*OLE*	$IC_3H_7O_2$
C_2H_6	*ALD2*	$HYPROPO_2$
C_2H_5OH	*ROOH*	*ROR*
C_3H_8	PAN	*RXPAR*
C_3H_6	*ONIT*	XO_2
C_5H_8	SO_2	XO_2N
$C_{10}H_{16}$	DMS	
CH_3COCHO	MSA	
CH_3COCH_3	NH_2	
CH_3OH	NH_3	
HCOOH	C_2O_3	
MCOOH	ISPD	

SO_4
$NO_3^{(A)}$
NH_4

Pseudo-aerosol species

(whole-atm species)

O_3	N_2O_5
OH	Rn
H_2O_2	
CO	
CH_2O	
CH_3O_2	
CH_3OOH	
CH_4	
NO	
NO_2	
NO_3	
HNO_3	
HO_2NO_2	

Stratospheric species (BASCOE)

O	HCl	CH_3Br	CFC-115
$O^{(1D)}$	HOCl	CH_2Br_2	HCFC-22
H	CH_3Cl	$CHBr_3$	HA-1301
H_2	CH_3CCl_3	$BrONO_2$	HA-1211
H_2O	CCL_4	BrO	
CH_3	$ClONO_2$	HBr	
CH_3O	$ClNO_2$	HOBr	
HCO	ClO	BrCl	
CO_2	OClO	HF	
N	ClOO	CFC-11	
N_2O	Cl_2O_2	CFC-12	
Cl	Br	CFC-113	
Cl_2	Br_2	CFC-114	

OCS
SO_3
H_2SO_4

Sulphur extensions

Coupling chemistries across the tropopause

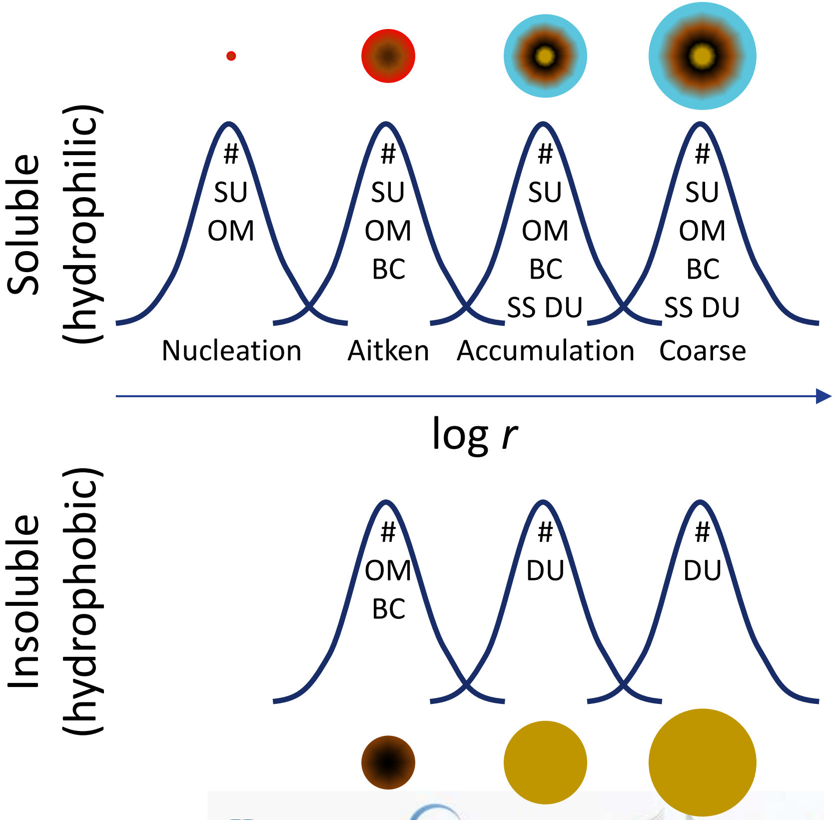
- CB05 reactions applied in troposphere
- BASCOE reactions applied in stratosphere
- Some reactions appear in both schemes
- Only one set of tracers, but some species are inert above or below the tropopause
- Lower boundary conditions prescribed for species only relevant in stratosphere
- "Chemical" tropopause defined:
  - troposphere where O3 < 200 ppb *and* CO > 40 ppb *and* p > 40 hPa
  - stratosphere elsewhere
- "Modified Band" photolysis in troposphere; LUT in stratosphere.

Structural differences between AER (bulk) and GLOMAP-mode

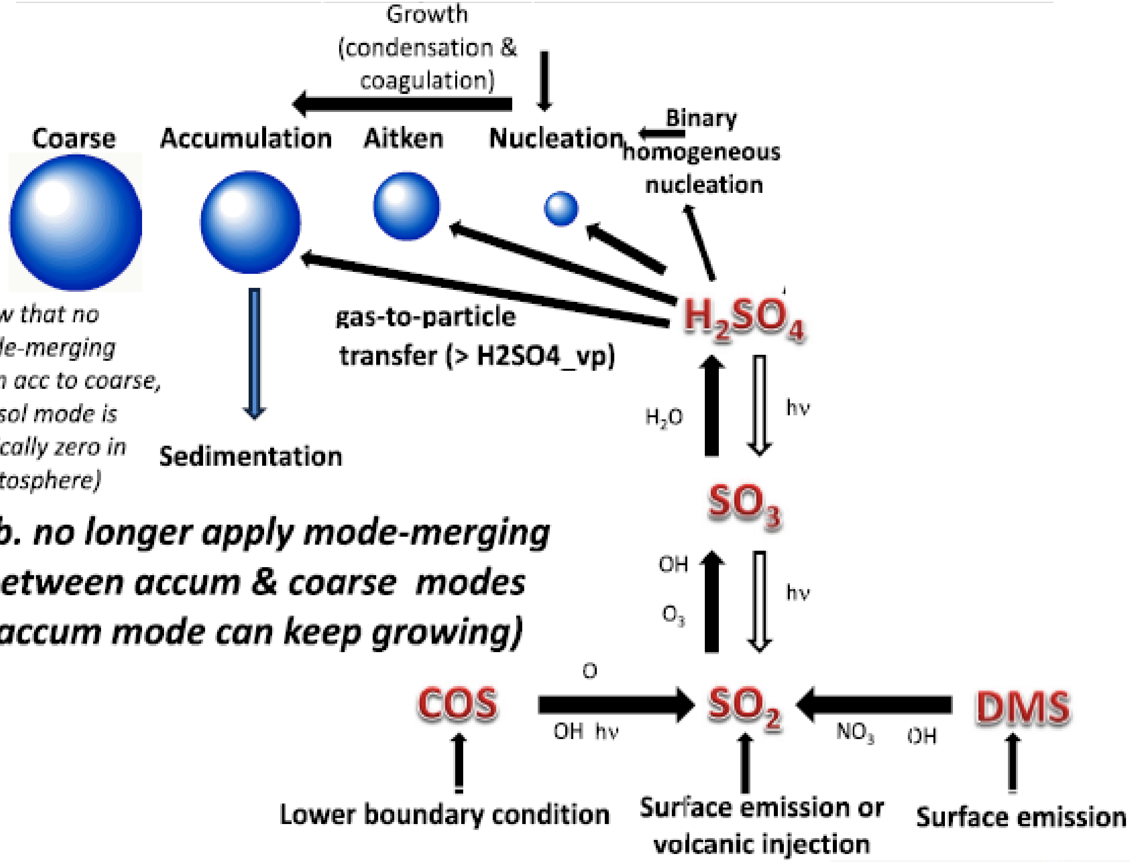
AER: 11/14 tracers

SS_{small}	SS_{mid}	SS_{large}
DU_{small}	DU_{mid}	DU_{large}
OM_{hphob}	OM_{hphil}	
BC_{hphob}	BC_{hphil}	
	SO_4	
$NO_{3\ fine}$	$NO_{3\ coarse}$	NH_4

GLOMAP-mode: 26 tracers



Stratosphere-enabled GLOMAP as implemented in the IFS



(Now that no mode-merging from acc to coarse, cor-sol mode is basically zero in stratosphere)

N.b. no longer apply mode-merging between accum & coarse modes (accum mode can keep growing)

Aerosol-chemistry interactions

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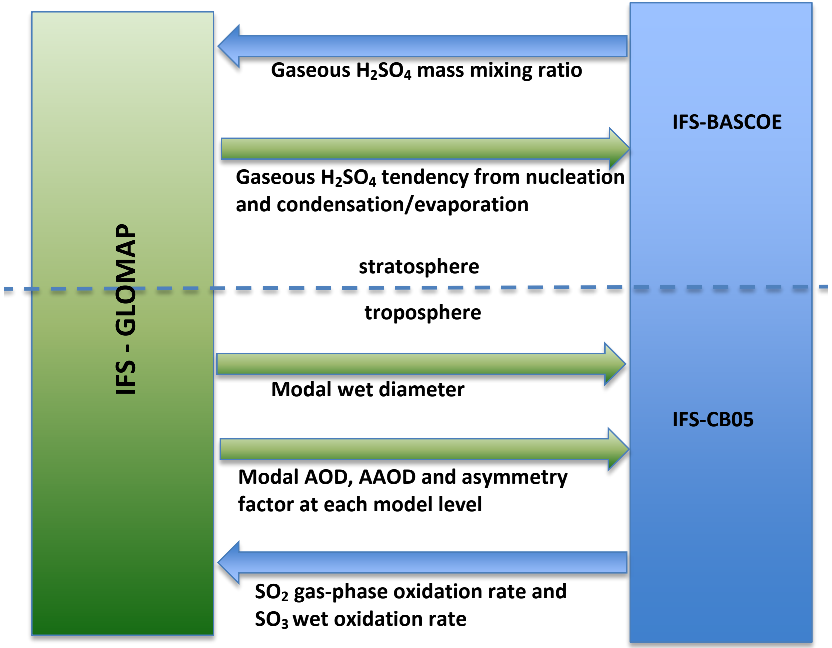
- Stratospheric sulphur cycle has been implemented in IFS-CB05-BASCOE
- Stratospheric coupling of IFS-CB05-BASCOE with IFS-GLOMAP
  - Sulphuric acid from IFS-BASCOE
  - Sulphuric acid tendencies from nucleation and condensation from IFS-GLOMAP
- Tropospheric coupling of IFS-CB05 with IFS-GLOMAP
  - SO_x oxidation rate from IFS-CB05
  - Aerosol wet diameter from IFS-GLOMAP to compute Surface Area Density (SAD) for heterogeneous chemical reactions
  - Aerosol optical properties to compute photolysis rates



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Sulfur chemistry in IFS(CB05-BASCOE)

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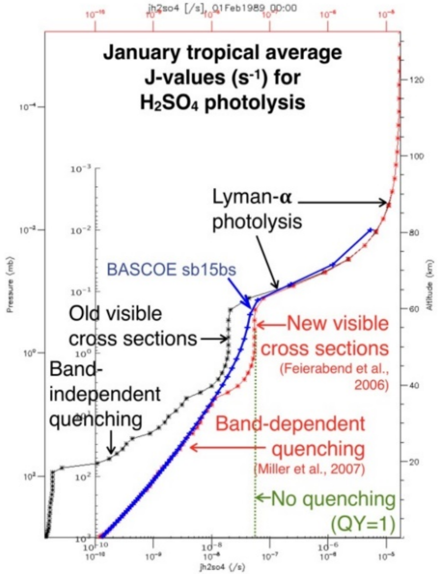
- Tropo (CB05): direct $SO_2 \rightarrow H_2SO_4$; DMS available ; OCS neglected
- Strato (BASCOE): sulfur chemistry added specifically for ICBG, as Dhomse *et al.* (2014) with rates from JPL 2015, including 3 photolyses:

Reaction	Rate expression
OCS + O → CO + SO_2	$2.1 \times 10^{-11} \exp(-2200/T)$
OCS + OH → CO_2 + SO_2	$7.2 \times 10^{-14} \exp(-1070/T)$
SO_2 + OH → SO_3 + HO_2	Third-body reaction (3.3x10^{-31},4.3, 1.6x10^{-12}, 0.)
SO_2 + O_3 → SO_3	$3.0 \times 10^{-12} \exp(-7000/T)$
SO_3 + H_2O → H_2SO_4	$8.5 \times 10^{-41} \exp\left(-\frac{6540}{T}\right) \cdot [H_2O]$
OCS + *hv* → CO + SO_2	(Burkholder et al. 2015)
H_2SO_4 + *hv* → SO_3 + H_2O	(see right)
SO_3 + *hv* → SO_2 + O	(Burkholder et al. 2015)



Photolysis of H_2SO_4 includes Lyman-α (Lane and Kjaergaard, 2008) and visible bands (Feierabend, 2006) with band-dependent quenching (Miller et al., 2007). Result in ICBG (blue line) similar to WACCM implementation (red line) except for lower values in upper strato.

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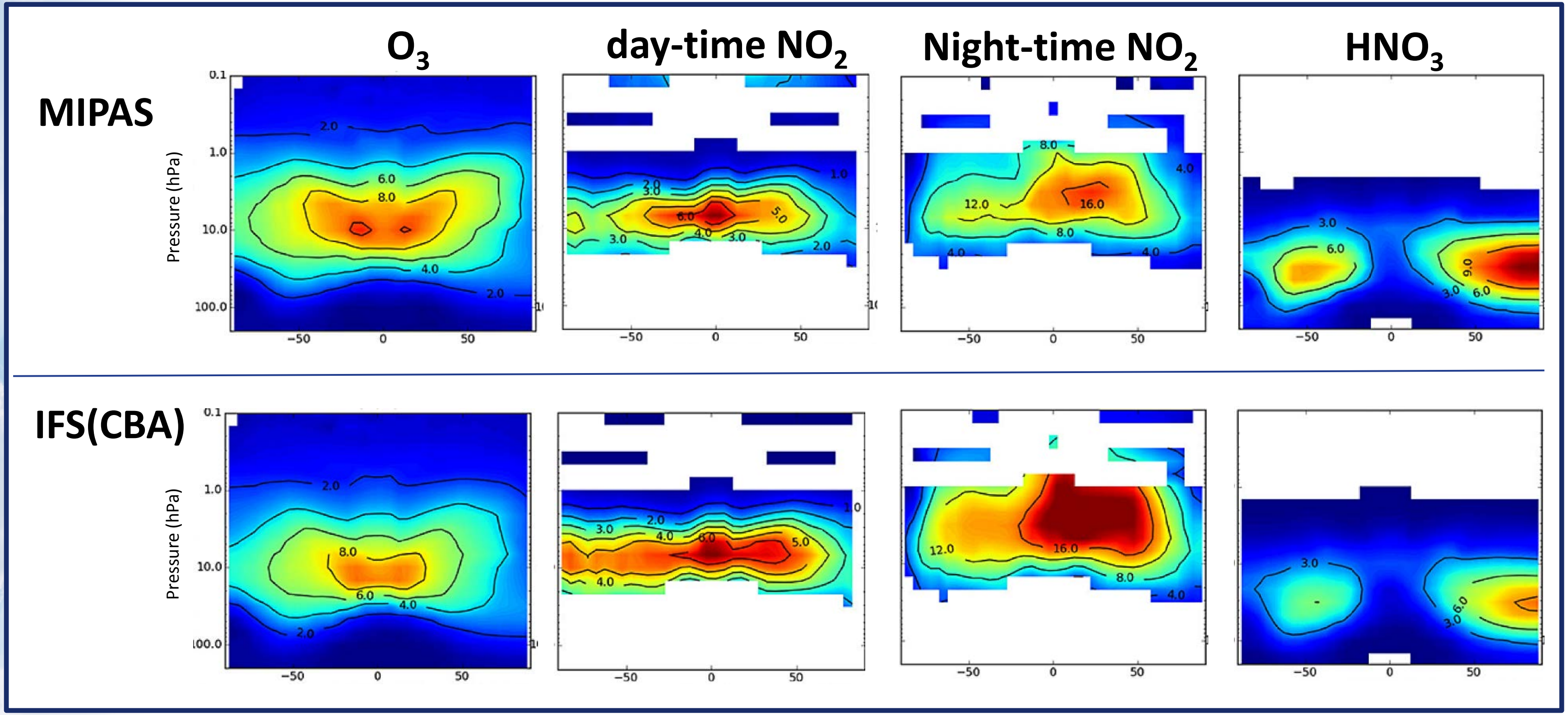
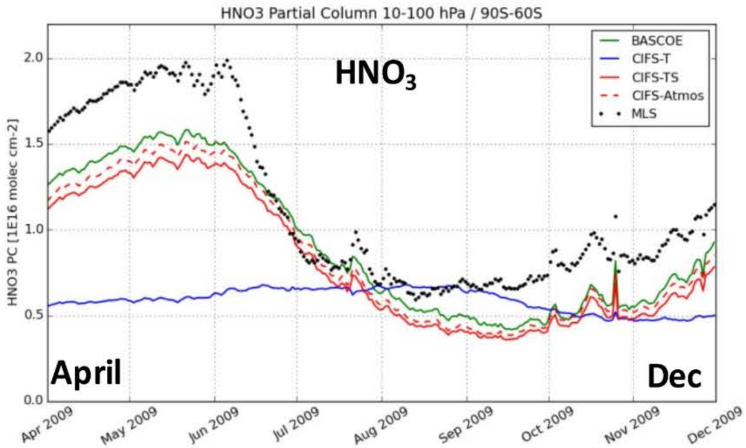
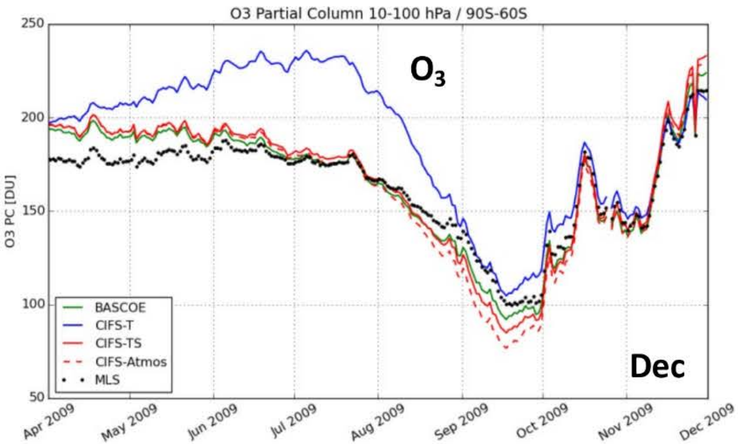
IFS-CB05-BASCOE stratosphere vs MIPAS

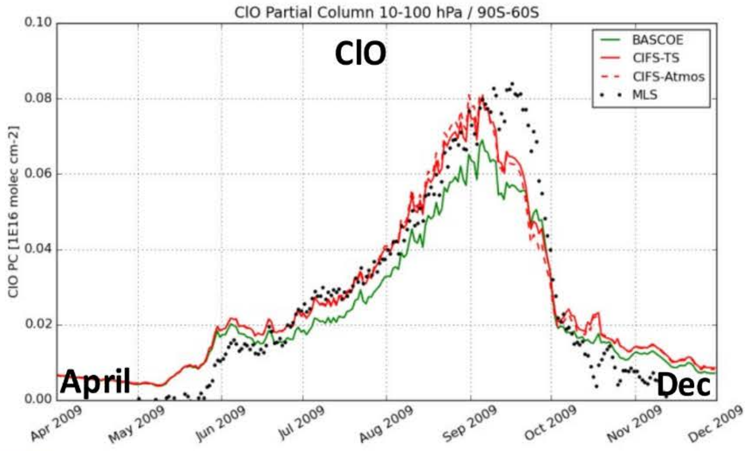


Monthly means for October 2009 (*Huijnen et al., GMD, 2016*)

Stratospheric chemistry during ozone hole conditions







- C-IFS-CB05
- C-IFS-CB05-BASCOE
- BASCOE-CTM
- MLS observations

Huijnen et al., GMD 2016

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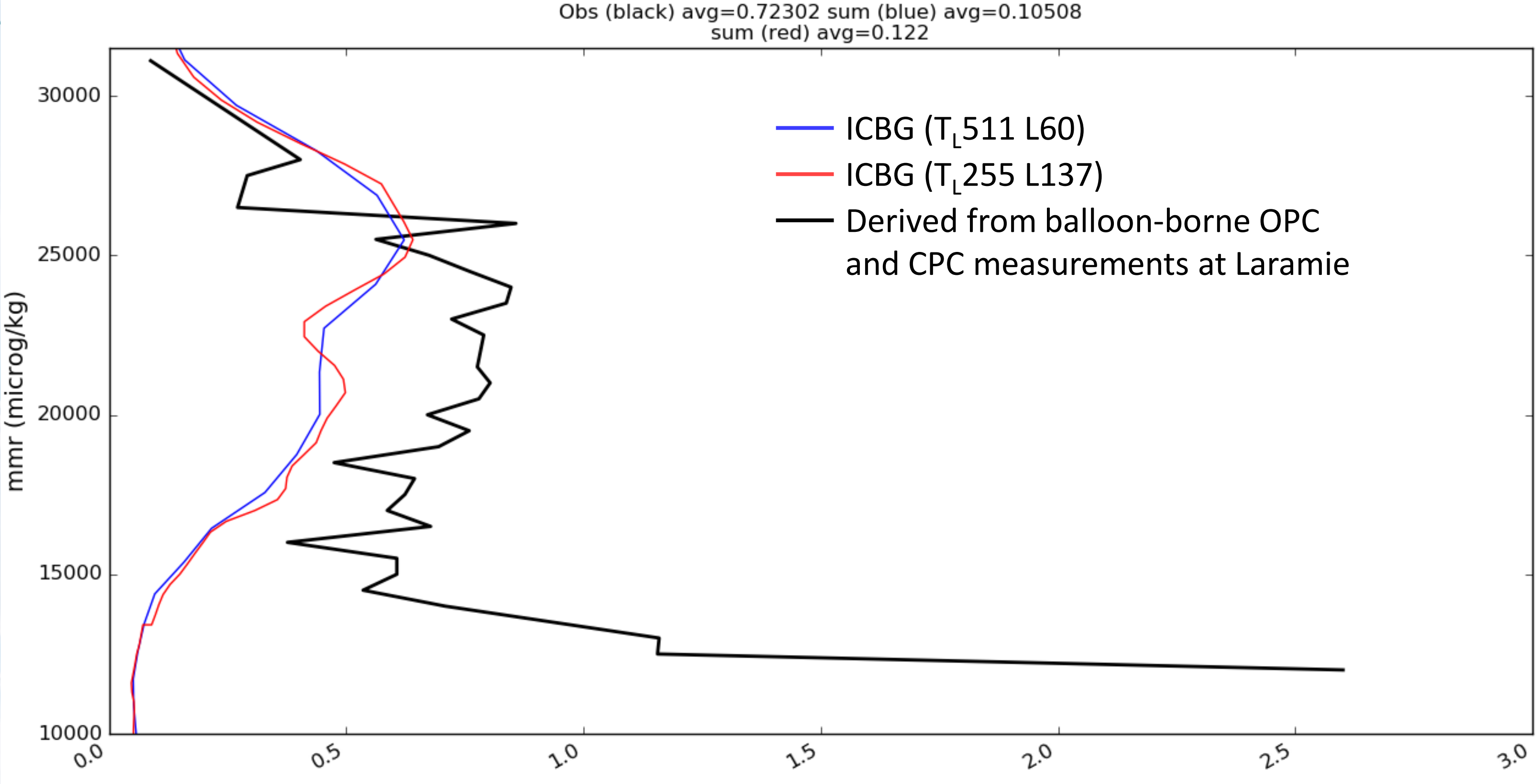
Preliminary evaluation of quiescent stratospheric sulphate aerosol



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Volcanic simulation: coupling of IFS-CB05-BASCOE with IFS-GLOMAP

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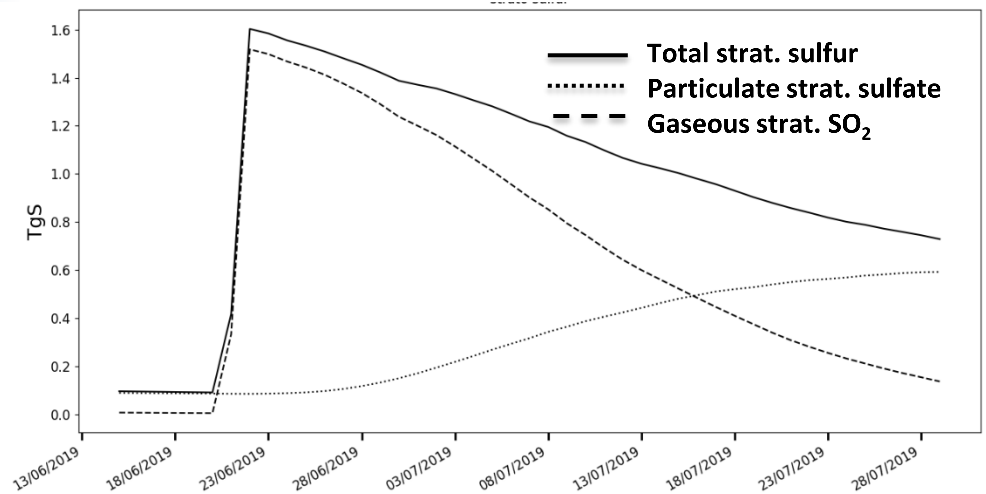
This new IFS-CB05-BASCOE-GLOMAP (ICBG) system has been tested on various volcanic events:

- Pinatubo (June 1991, ~14Tg SO_2 release)
- Calbuco (April 2015, ~0.4 Tg SO_2 release)
- Raikoke (June 2019, ~1.5 Tg SO_2 release)



Time evolution of simulated global stratospheric total, particulate and gaseous sulfur during the Raikoke eruption (using a 3Tg release of SO_2 on 21/22 June 2019)

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Follow-up of simulations of Pinatubo eruption: SO_2 and sulfate

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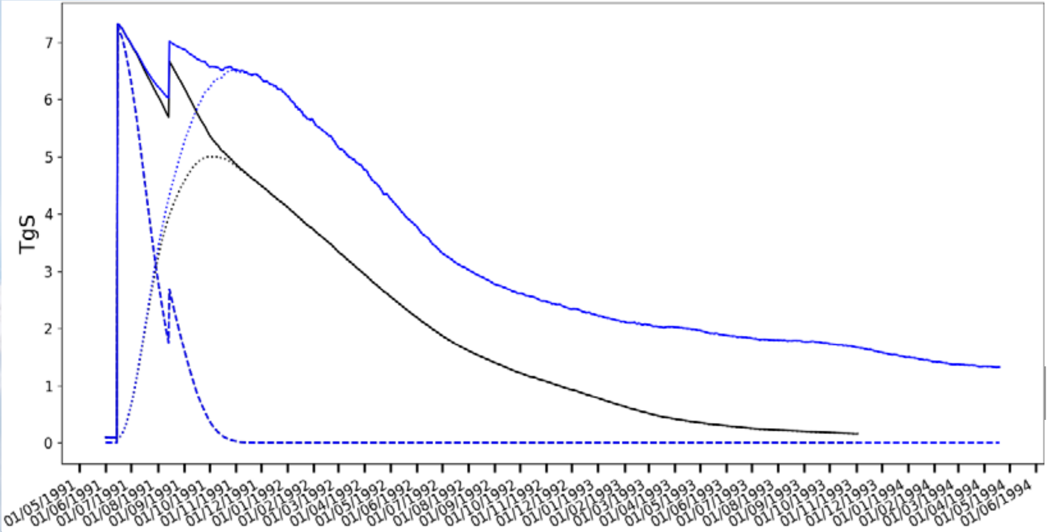
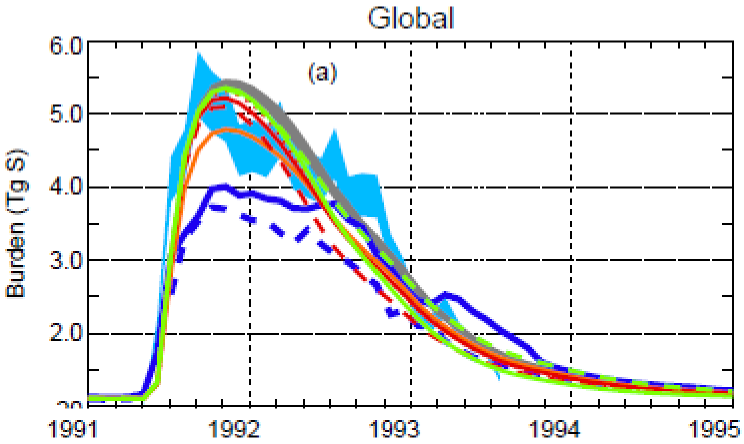
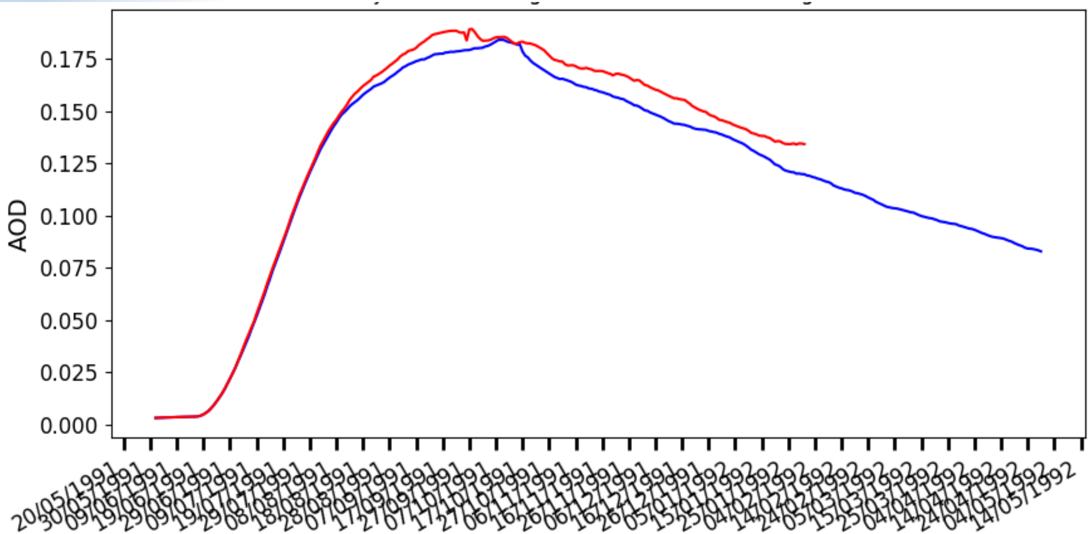


Stratospheric SO2 (dashed line), sulfate (dotted line) and total sulphur (solid line). Black: IFS-AER sedimentation, blue, “explicit” sedimentation

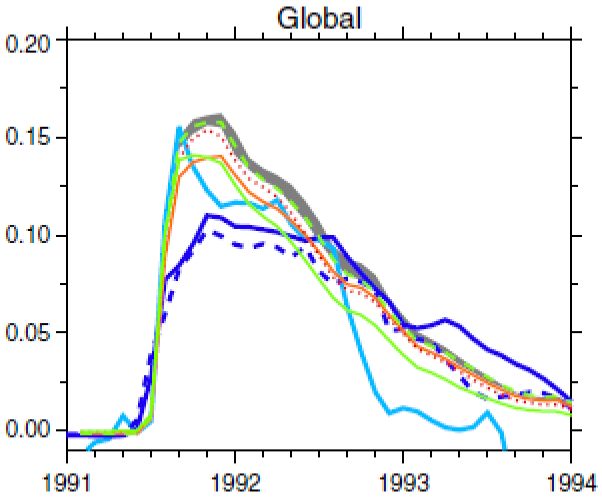


Stratospheric particulate sulphate from Sukhodolov et al. (2018). Light/dark blue = retrievals.

Follow-up of simulations of Pinatubo eruption: sAOD



Stratospheric AOD at 550 nm, sedimentation from IFS-AER (blue) and "explicit" sedimentation (red)



Stratospheric AOD from Sukhodolov et al. (2018). Light/dark blue = retrievals.

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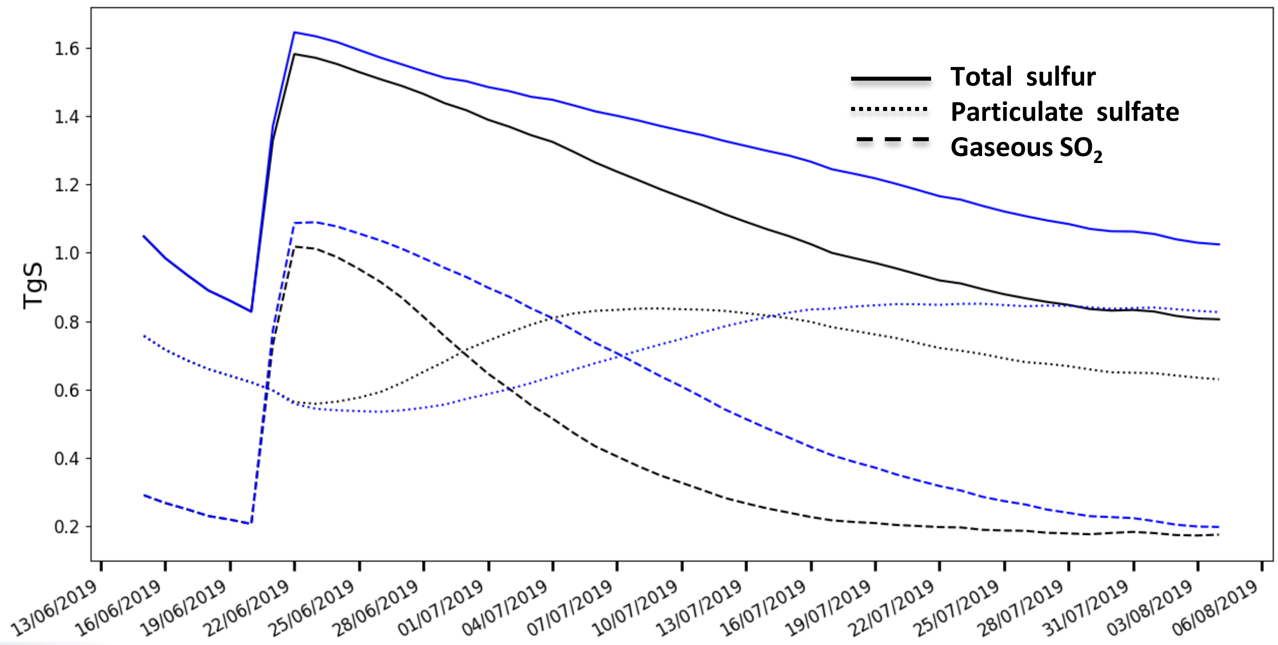
ICBG used for Raikoke eruption case study

1.5Tg SO_2 release at 7-15km and 13-16km



Time evolution of simulated global total, particulate and gaseous sulfur during the Raikoke eruption using a 1.5Tg release of SO_2 on 21/22 June 2019) . Black, release at 7-15 km; blue, release at 13-16 km

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Volcanic simulation: coupling of IFS-CB05-BASCOE with IFS-GLOMAP

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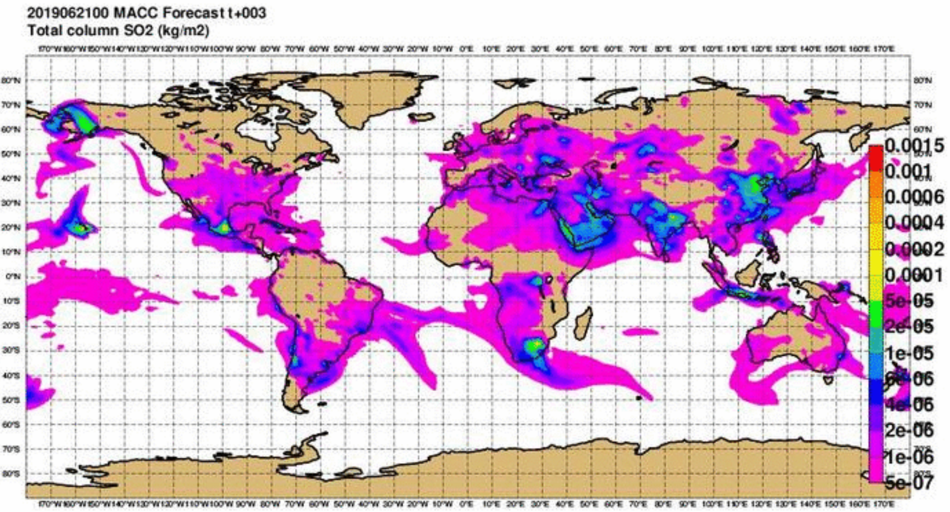
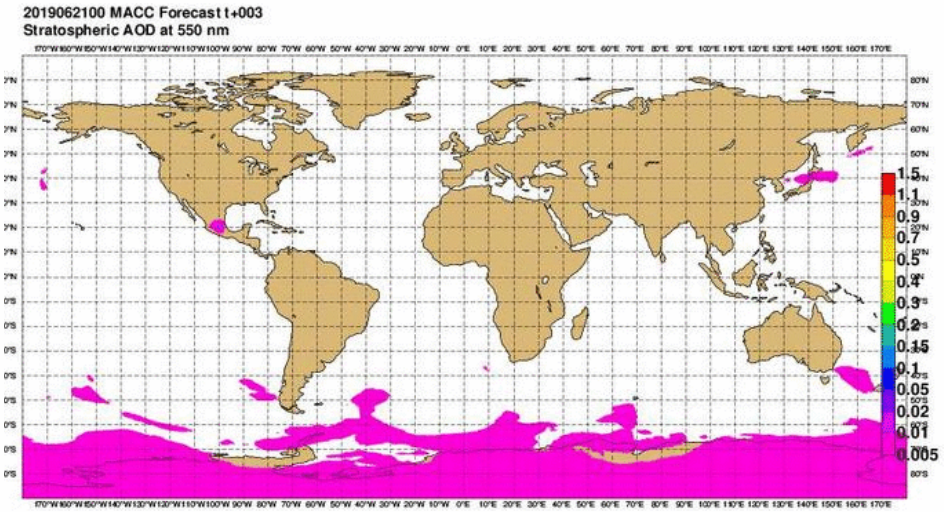
Simulation of the Raikoke eruption on 21/22 June 2019





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Further developments

- Coupling GLOMAP surface area density to stratospheric chemistry.
- Further evaluation of both quiescent state and volcanic response.
- Porting newer GLOMAP extensions (nitrates, meteoric smoke etc.)
- Fixing technical issues, numerical instabilities etc.
- Extending 4D-Var data assimilation to ICBG:
  - Largely working in respect of CB05–BASCOE chemistry [O_3, CO, NO_2, (volcanic) SO_2, CH_2O (passive monitoring only)]
  - Basic implementation in place for GLOMAP aerosol, but technical and numerical issues remain