

# 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** 2017

**Project Title:** Inline chemistry for tropospheric and stratospheric trace gases in IFS

**Computer Project Account:** SPNLMACC

**Principal Investigator(s):** Dr. V. Huijnen

**Affiliation:** Royal Netherlands Meteorological Institute (KNMI)

**Name of ECMWF scientist(s) collaborating to the project**  
(if applicable) J. Flemming

**Start date of the project:** 2015

**Expected end date:** 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
<b>High Performance Computing Facility</b>	(units)	1200k	1176k	1400k	371k
<b>Data storage capacity</b>	(Gbytes)				

## Summary of project objectives

(10 lines max)

Composition-IFS where CB05 tropospheric chemistry is integral part of the IFS code, allows unprecedented couplings between chemical tracer fields with aerosol and meteorological aspects. The aims of the current special project are (i) to extend the existing chemical scheme, by introducing stratospheric chemistry from the BASCOE scheme, and (ii) to optimize the solver, through the use of a pre-processor, and (iii) to explore new interactions specifically related to the new aerosol model. This aims to support the work performed in the MACC-III and scientific aspects related to the more operational tasks done in the framework of the Copernicus Atmospheric Monitoring Service.

## Summary of problems encountered (if any)

(20 lines max)

No significant problems have occurred

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

Benchmarking of the BASCOE stratospheric chemistry module as implemented in the IFS, has been finalized, and shown to work well in terms of stratospheric ozone, and its ability to capture the ozone hole chemistry (Huijnen et al., 2016a). Also model performance of related (precursor) trace gases has been extensively documented, and evaluation tools form the basis for further analysis of different chemistry implementations of C-IFS, as developed during the Copernicus tender CAMS\_42.

Development efforts have shifted towards exploratory testing and further integration of chemistry aspects that affect the aerosol: the inorganic aerosol module (sulfate, ammonium, nitrate) and organic aerosol (secondary aerosol formation).

### *Inorganic aerosol*

The existing inorganic aerosol parameterization has been checked by evaluating the production and loss budget terms. This has led to revision of the dry deposition velocity (it was too high), and wet removal (also too high). While aerosol dry deposition has currently be scaled down by a simple tuning factor (a more detailed revision of dry deposition parameterization is planned for upcoming year, as part of the CAMS\_42 tender), the aerosol wet deposition parameterization has been checked and revised. For this, the in-cloud scavenging coefficients  $C$  have been modified, according to Bourgeois and Bey, (JGR 2011), by making distinction between stratiform ice, mixed and liquid clouds. For below-cloud scavenging Croft et al., (ACP 2009) serves as reference. For rain, scavenging coefficients of  $1 \times 10^{-3} \text{ m}^2 \text{ kg}^{-1}$  is assumed, for snow a loss of  $5 \times 10^{-3} \text{ m}^2 \text{ kg}^{-1}$ .

Both updates on in-cloud and below-cloud scavenging lead to lower aerosol removal rate, and, together with the lower dry deposition rates this consequently results in larger aerosol lifetimes (~4 days, rather than 1 day in the previous setup). Hence this leads to considerable changes in the sulfate, ammonium and nitrate burdens as modelled in the chemistry scheme, which brings them closer to the variants available in the aerosol scheme. Also the equilibrium approach for ammonium and nitrate aerosol, based on EQSAM, has been verified and checked against the corresponding parameterization available from the existing aerosol module in CAMS, referred to as INCA. This activity hence serves to align and integrate the aerosol and chemistry modules in IFS.

### *Secondary organic aerosol*

June 2017

This template is available at:  
<http://www.ecmwf.int/en/computing/access-computing-facilities/forms>

## Secondary organic aerosol

A new module to describe efficiently the secondary organic aerosol (SOA) production linked to chemistry precursors is in development. This involves irreversible formation (from methyl glyoxal (MGLY) conversion in cloud droplets), as well as reversible formation. Here gas-phase VOC's are assumed in equilibrium with aerosol, depending on the volatility of the respective molecule. The purpose is to replace the currently existing parameterization of SOA, based on a presumed SOA formation of  $\sim 100 \text{ Tg yr}^{-1}$  for anthropogenic sources, following the spatial and temporal distribution of CO anthropogenic emissions, and  $\sim 18 \text{ Tg}$  of biogenic sources, to allow for a more dynamical description of SOA formation which better describes the physical and chemical processes involved. Here we present the latest status, but note that this is still work-in-progress.

In the current implementation we keep track of four individual SOA tracers:

- (1) SOA produced from MGLY irreversible conversion (SOA-MGLY)
- (2) biogenic SOA, produced from terpene and isoprene oxidation with OH and O<sub>3</sub> (bSOA)
- (3) anthropogenic SOA produced from OLE, PAR and C<sub>3</sub>H<sub>6</sub> oxidation with OH and O<sub>3</sub> (aSOA)
- (4) biogenic/anthropogenic SOA produced from volatile organic nitrate compounds (onSOA).

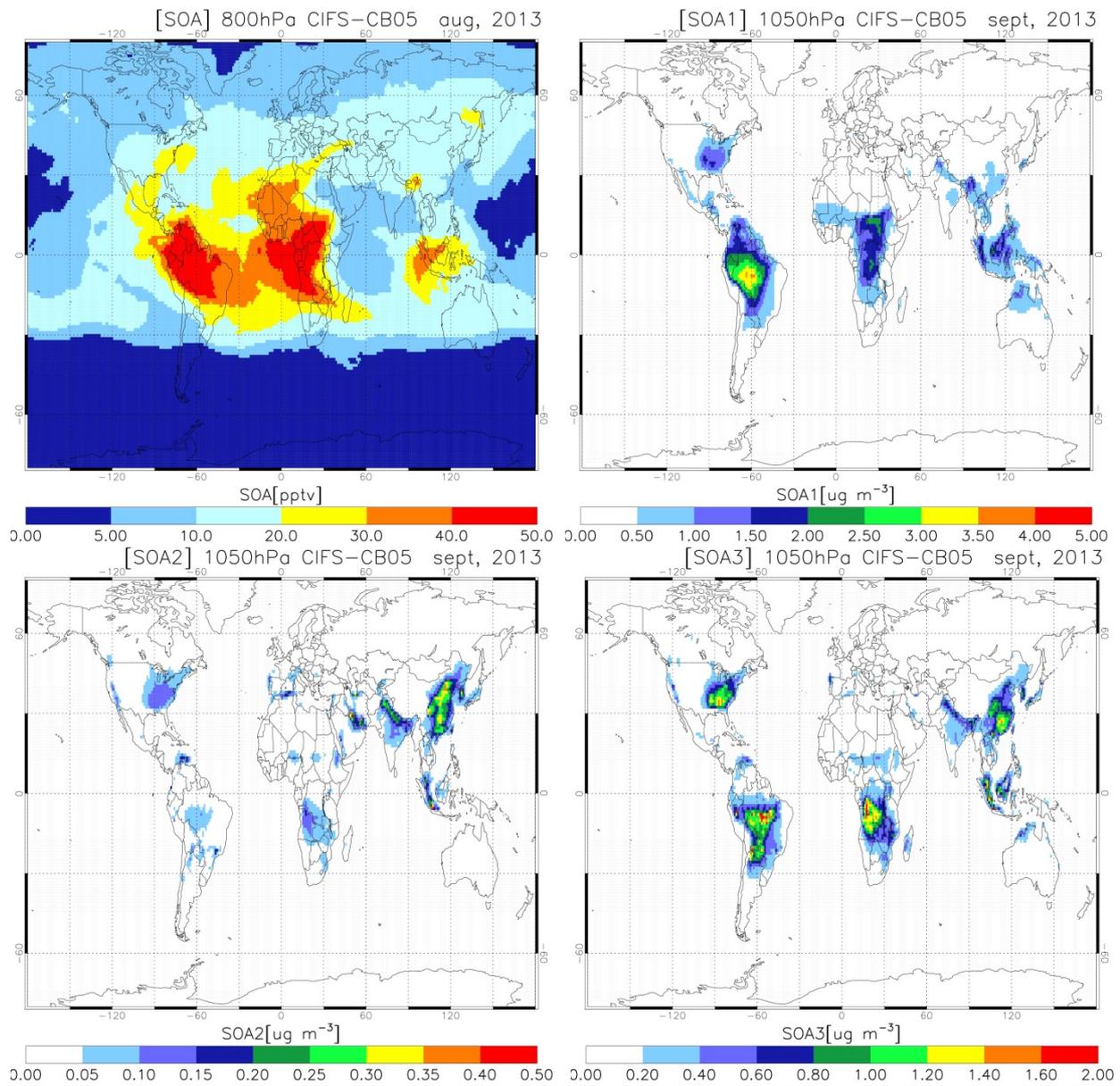
For the bSOA and aSOA corresponding secondary organic gas-phase precursors (SOGs) are described, which are formed from the oxidation reactions of the precursor gases with OH and O<sub>3</sub>. These SOG tracers are also subject to wet deposition. Currently only single volatilities are assumed for each of the SOA tracers, following recommendations described in Tsimpidi et al. (GMD2014).

Table 1. Annual budgets of various SOA tracers as implemented in C-IFS

Term	Production (Tg/yr)	Burden (Tg)	Lifetime (days)
SOA-MGLY	16	0.27	5.9
bSOA	28	0.65	8.3
aSOA	3.0	0.08	10.0
onSOA3	20.	0.31	5.9

Note that the production budget on average equals the loss through wet deposition, and that currently no dry deposition and/or sedimentation in place for the SOA tracers. Figure 1 shows an indication of the spatial distribution and magnitudes of the various SOA tracers.

Table 1 provides an overview of current annual production, and global burdens. The total annual SOA production is  $\sim 67 \text{ Tg yr}^{-1}$ . From this, about  $4 \text{ Tg yr}^{-1}$  can be attributed to anthropogenic sources ( $3.0 \text{ Tg yr}^{-1}$  from PAR, OLE and C<sub>3</sub>H<sub>6</sub> + O<sub>3</sub>/OH, and about  $1 \text{ Tg yr}^{-1}$  from organic nitrate). In comparison, Tsimpidi et al. (2014), their Table 7, report a total burden of biogenic SOA of 0.55 Tg (bSOA-v) and 0.65 Tg anthropogenic SOA (aSOA-v), i.e. our current model version is slightly higher for biogenic, but significantly lower in terms of anthropogenic SOA. This points to the fact of missing anthropogenic emission sources (specifically xylene, toluene), while also in the current implementation, using a single volatility bin is assumed no ageing is modelled. Tsimpidi et al (2014) have pointed out that in fact for anthropogenic precursors this is an important source of organic aerosol.



*Figure 1: SOA-MGLY at 800hPa (top left), as well as surface distributions of bSOA (top right), aSOA (bottom left) and noSOA(bottom right), all averaged over September 2013.*

## List of publications/reports from the project with complete references

- Eskes, H., Huijnen, V., Arola, A., Benedictow, A., Blechschmidt, A.-M., Botek, E., Boucher, O., Bouarar, I., Chabrillat, S., Cuevas, E., Engelen, R., Flentje, H., Gaudel, A., Griesfeller, J., Jones, L., Kapsomenakis, J., Katragkou, E., Kinne, S., Langerock, B., Razinger, M., Richter, A., Schultz, M., Schulz, M., Sudarchikova, N., Thouret, V., Vrekoussis, M., Wagner, A., and Zerefos, C.: Validation of reactive gases and aerosols in the MACC global analysis and forecast system, *Geosci. Model Dev.*, 8, 3523-3543, doi:10.5194/gmd-8-3523-2015, 2015.
- Flemming, J., Huijnen, V., Arteta, J., Bechtold, P., Beljaars, A., Blechschmidt, A.-M., Diamantakis, M., Engelen, R. J., Gaudel, A., Inness, A., Jones, L., Josse, B., Katragkou, E., Marecal, V., Peuch, V.-H., Richter, A., Schultz, M. G., Stein, O., and Tsikerdekis, A.: Tropospheric chemistry in the Integrated Forecasting System of ECMWF, *Geosci. Model Dev.*, 8, 975-1003, doi:10.5194/gmd-8-975-2015, 2015.
- Huijnen, V., Flemming, J., and Errera, Q., Updated documentation of C-IFS-CB05 and C-IFS-CB05-BASCOE. MACC-III Technical report D24.1, 2015.
- Huijnen, V., Flemming, J., Chabrillat, S., Errera, Q., Christophe, Y., Blechschmidt, A.-M., Richter, A., and Eskes, H.: C-IFS-CB05-BASCOE: stratospheric chemistry in the Integrated Forecasting System of ECMWF, *Geosci. Model Dev.*, 9, 3071-3091, doi:10.5194/gmd-9-3071-2016, 2016a.
- Huijnen, V., M. J. Wooster, J. W. Kaiser, D. L. A. Gaveau, J. Flemming, M. Parrington, A. Inness, D. Murdiyarmo, B. Main and M. van Weele. Fire carbon emissions over maritime southeast Asia in 2015 largest since 1997. *Sci. Rep.* 6, 26886; doi: 10.1038/srep26886, 2016b.
- Inness, A., Blechschmidt, A.-M., Bouarar, I., Chabrillat, S., Crepulja, M., Engelen, R. J., Eskes, H., Flemming, J., Gaudel, A., Hendrick, F., Huijnen, V., Jones, L., Kapsomenakis, J., Katragkou, E., Keppens, A., Langerock, B., de Mazière, M., Melas, D., Parrington, M., Peuch, V. H., Razinger, M., Richter, A., Schultz, M. G., Suttie, M., Thouret, V., Vrekoussis, M., Wagner, A., and Zerefos, C.: Data assimilation of satellite-retrieved ozone, carbon monoxide and nitrogen dioxide with ECMWF's Composition-IFS, *Atmos. Chem. Phys.*, 15, 5275-5303, doi:10.5194/acp-15-5275-2015, 2015.
- Inness, A., Benedetti, A., Flemming, J., Huijnen, V., Kaiser, J. W., Parrington, M., and Remy, S.: The ENSO signal in atmospheric composition fields: emission-driven versus dynamically induced changes, *Atmos. Chem. Phys.*, 15, 9083-9097, doi:10.5194/acp-15-9083-2015, 2015.

## Summary of plans for the continuation of the project

(10 lines max)

In the last half year of this special project we plan to further develop the implementation of the inorganic and organic aerosol coupling with chemistry precursors. While this should lead towards operational application of the inorganic couplings, for the organic aerosol we foresee that further work is needed in terms of model evaluation, and selecting the most appropriate setup. Specifically, a balance between level of detail of the modelling, and efficiency for running in operational system needs to be defined that is useful in the framework of CAMS.