SPECIAL PROJECT PROGRESS REPORT

All the following mandatory information needs to be provided. The length should *reflect the complexity and duration* of the project.

Reporting year	2018
Project Title:	Chemistry and aerosol processes modelling within IFS in extension to CAMS activities
Computer Project Account:	SPNLMACC
Principal Investigator(s):	V. Huijnen
Affiliation:	Royal Netherlands Meteorological Institute (KNMI)
Name of ECMWF scientist(s) collaborating to the project (if applicable)	N/A
Start date of the project:	2018
Expected end date:	2020

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)	1500	258	1700	0
Data storage capacity	(Gbytes)				

Summary of project objectives (10 lines max)

Within the Copernicus Atmosphere Monitoring Service (CAMS) modules for tropospheric and stratospheric chemistry, integrated in ECMWF's Integrated Forecasting System (IFS), are maintained and further improved within the CAMS tender on reactive gases modelling and assimilation, but does not cover extended scientific spinoff's from this work. This special project aims to provide us with in the computer resources needed for this. Topics under consideration are: 1) a further integration of tropospheric and stratospheric chemistry; 2) further integration of chemistry and aerosol subjects, particularly stratospheric aerosol and secondary organic aerosol; 3) Re-evaluate specific case studies, particularly the 2015 Indonesian fires. This special project is a follow-up of the previous one (2015-2017).

Summary of problems encountered (10 lines max)

No significant problems have occurred. Only limited resources have been used on account of this special project, and some activities have been postponed in alignment with particular CAMS project deliverables. Also developments have been accounted for through dedicated CAMS budget.

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

In the third year of this special project we plan to evaluate more closely the stratospheric composition, with focus on CH_4 and H_2O. Also further develop the implementation of the inorganic and organic aerosol coupling with chemistry precursors, in particular for the organic aerosol further work is needed in terms of model tuning and evaluation.

List of publications/reports from the project with complete references

Banda et al., Monitoring emissions from the 2015 Indonesian fires using CO satellite data, Phil. Trans. Royal Soc. B: Biological Sciences 373(1760), 2018.

Hall, S. R., Ullmann, K., Prather, M. J., Flynn, C. M., Murray, L. T., Fiore, A. M., Correa, G., Strode, S. A., Steenrod, S. D., Lamarque, J.-F., Guth, J., Josse, B., Flemming, J., Huijnen, V., Abraham, N. L., and Archibald, A. T.: Cloud impacts on photochemistry: building a climatology of photolysis rates from the Atmospheric Tomography mission, Atmos. Chem. Phys., 18, 16809-16828, https://doi.org/10.5194/acp-18-16809-2018, 2018.

Huijnen, V., M. J. Wooster, J. W. Kaiser, D. L. A. Gaveau, J. Flemming, M. Parrington, A. Inness, D. Murdiyarso, 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, 2016.

Huijnen, V., Pozzer, A., Arteta, J., Brasseur, G., Bouarar, I., Chabrillat, S., Christophe, Y., Doumbia, T., Flemming, J., Guth, J., Josse, B., Karydis, V. A., Marécal, V., and Pelletier, S.: Quantifying uncertainties due to chemistry modelling – evaluation of tropospheric composition simulations in the CAMS model (cycle 43R1), Geosci. Model Dev., 12, 1725-1752, https://doi.org/10.5194/gmd-12-1725-2019, 2019.

Inness, A., Ades, M., Agustí-Panareda, A., Barré, J., Benedictow, A., Blechschmidt, A.-M., Dominguez, J. J., Engelen, R., Eskes, H., Flemming, J., Huijnen, V., Jones, L., Kipling, Z., Massart, S., Parrington, M., Peuch, V.-H., Razinger, M., Remy, S., Schulz, M., and Suttie, M.: The CAMS reanalysis of atmospheric composition, Atmos. Chem. Phys., 19, 3515-3556, https://doi.org/10.5194/acp-19-3515-2019, 2019.

Rémy, S., Kipling, Z., Flemming, J., Boucher, O., Nabat, P., Michou, M., Bozzo, A., Ades, M., Huijnen, V., Benedetti, A., Engelen, R., Peuch, V.-H., and Morcrette, J.-J.: Description and evaluation of the tropospheric aerosol scheme in the Integrated Forecasting System (IFS-AER, cycle 45R1) of ECMWF, Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2019-142, in review, 2019.

Sander, R., Baumgaertner, A., Cabrera-Perez, D., Frank, F., Gromov, S., Grooß, J.-U., Harder, H., Huijnen, V., Jöckel, P., Karydis, V. A., Niemeyer, K. E., Pozzer, A., Riede, H., Schultz, M. G., Taraborrelli, D., and Tauer, S.: The community atmospheric chemistry box model CAABA/MECCA-4.0, Geosci. Model Dev., 12, 1365-1385, https://doi.org/10.5194/gmd-12-1365-2019, 2019.

Wooster, M.J., Gaveau, D.L.A., Salim, M.A., Zhang, T., Xu, W., Green, D.C., Huijnen, V., Murdiyarso, D., Gunawan, D., Borchard, N., Schirrmann, M., Main, B., Sepriando, A. New tropical peatland gas and particulate emissions factors indicate 2015 Indonesian fires released far more particulate matter (but Less Methane) than current inventories imply. Remote Sensing, 10 (4), 2018.

Summary of results (from January 2018 to June 2019)

During this phase of the project we have not started new activities, but consolidated various developments leading to several publications and manuscripts in preparation / in review. Here we provide a short overview of the most relevant results from the various manuscripts, and explain the contributions to them from this Special Project, and its precursor Special Project.

Banda et al. (2018) investigate a best-estimate of CO (and CO_2) emissions originating from the 2015 fires over Indonesia we based on a 4D-Var inversion system. For this study we ran several IFS model experiments with different emission estimates and assessed the impact on OH. This defines the lifetime of CO, and is hence an important, yet uncertain, parameter in inversion studies. Wooster et al., (2018) present in situ measurements to derive new PM2.5 emissions factors (EFs) for these Indonesian fires, along with updated EFs for a series of trace gases and physio-chemical measurements of the peatland fuel. Based on this, they provide new estimates of aerosol total emissions, also relying on total CO emissions from the Huijnen et al. (2016) study.

General chemistry model developments for the IFS(CB05) configuration have been used in the CAMS Reanalysis, published in 2018 (Inness et al., 2019). More recent updates to the system are made available in the pre-operational configurations of the CAMS system. In particular, Huijnen et al. (2019) report on the performance of the combined IFS(CB05BASCOE) system, with focus on the tropospheric composition. Remy et al., (2019) report on the aerosol module in CAMS, and show the importance of inorganic (and organic) chemistry precursors for the aerosol.

Recently more focus has indeed been given to the performance of the inorganic aerosol (sulfate and nitrate), with special attention to its performance to model deposition fluxes. In the following figures we provide a short evaluation of various aspects on this. Deposition of SO_2, the gaseous precursor for sulfate aerosol, is evaluated against CASTNET data for a simulation for 2005, see Figure 1. This shows that the general features are captured, with higher deposition fluxes over the (more densely populated) Eastern US, and less over the Western US. Still, the modeled dry deposition appears over-estimated, mainly because the near-surface concentrations of SO2 are over-estimated.
Evaluation of the sulfate dry and wet deposition is given in Figure 2. While deposition fluxes are captured over the Western US, they are generally under-estimated over the Eastern US. This appeared related to an under-estimate of SO_4 near-surface concentrations. This discrepancy compared to the findings for SO_2 needs further investigation, and could be associated to absence of injection height for SO_2 emissions (as compared to uncertainty in the emissions themselves). A first

evaluation of NH_4 deposition (Figure 3) shows values which are overall in the range of the observations for dry deposition, while an underestimate is found for wet deposition, mostly over the Eastern US. Ongoing activities in the remainder of this special project will focus on reducing these biases.

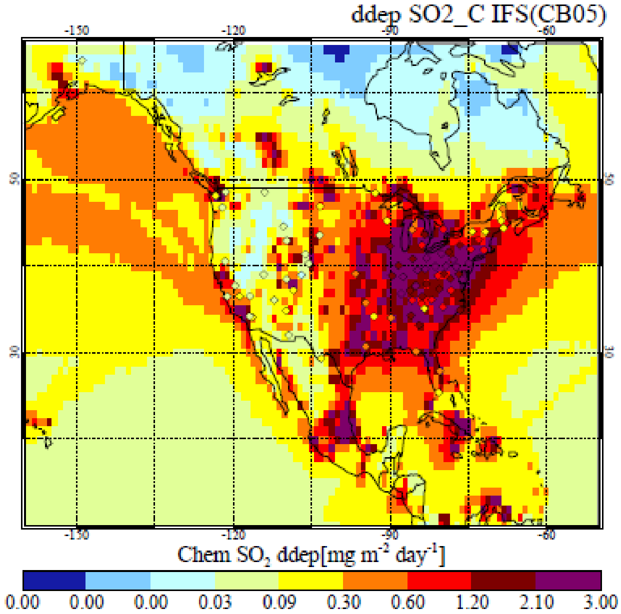

Figure 1: Modelled SO_2 dry deposition, evaluated against CASTNET data for 2005 (circles overlay)

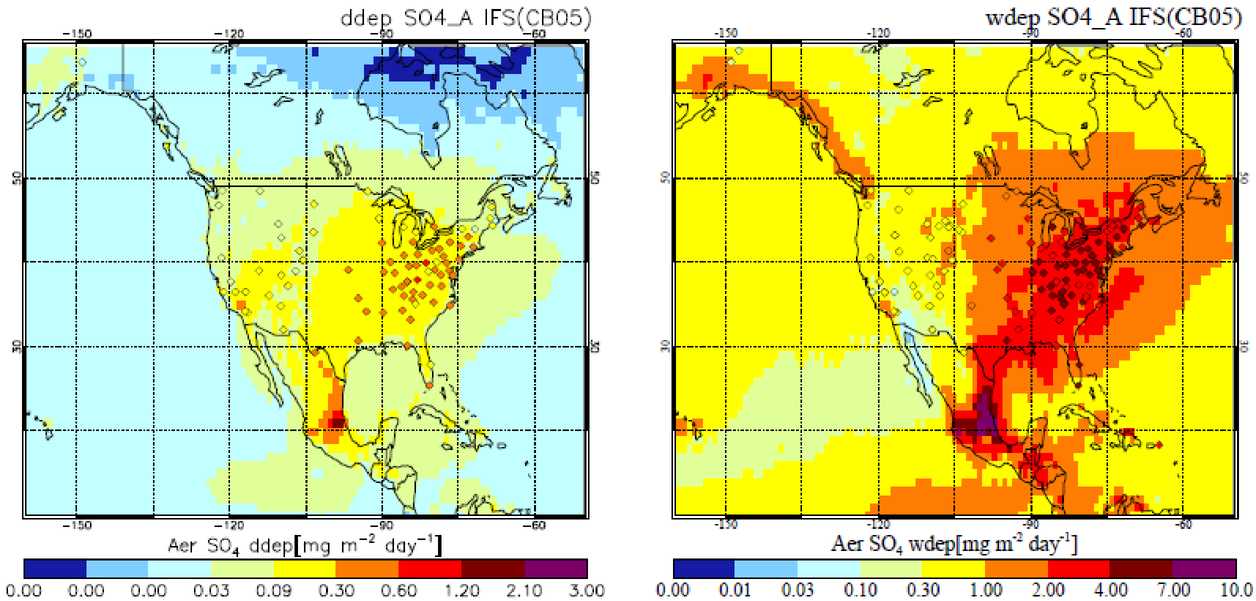

Figure 2: Modelled sulfate aerosol dry (left) and wet (right) deposition, evaluated against CASTNET data for 2005 (circles overlay)

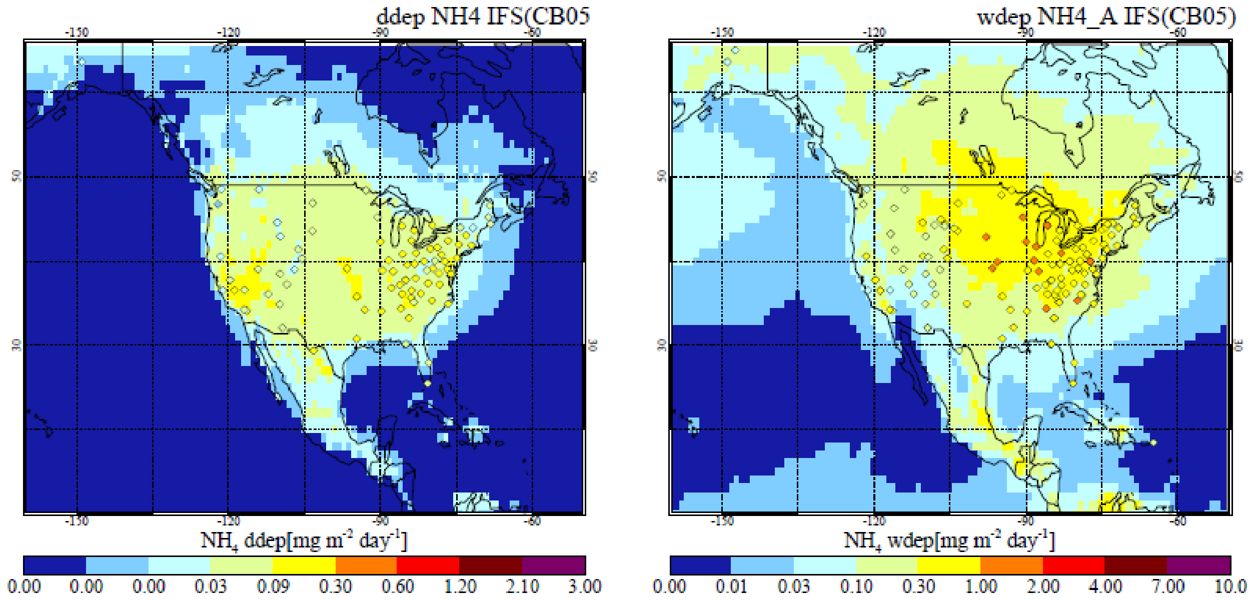

Figure 3: Modelled Ammonium dry (left) and wet (right) deposition, evaluated against CASTNET data for 2005 (circles overlay)