

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 2016

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
High Performance Computing Facility	(units)	1400k	1014k	800k	600k
Data storage capacity	(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 possibly forthcoming projects 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)

This section should comprise 1 to 8 pages and can be replaced by a short summary plus an existing scientific report on the project

During the last year work was performed mainly on the benchmarking of the stratospheric chemistry in the IFS, as documented in a paper currently in review in *Geosci. Model Dev.* (Huijnen et al., 2016a). Important elements are its current performance in terms of stratospheric ozone, and specifically the ability to capture the ozone hole situation. During the review status the PSC-parameterization has been questioned, and based on that this scheme has been revised and newly evaluated.

Also potential trends (biases) in O₃, and long-lived trace gases such as N₂O, CFC's, CH₄, which tend to develop in simulations exceeding 1 year length are assessed in multiple runs starting in 2008, and running through until 2010. Finally, the efficient approach where tropospheric and stratospheric chemistry have been resolved in their respective domains has been compared to a system which includes all reactions throughout the atmosphere. These runs have been computationally rather expensive, but turned out necessary and useful to assess the system.

Evaluation of current ability of the system

The performance of C-IFS-CB05-BASCOE and C-IFS-Atmos has been compared against observations from ozone sondes. For this a run initialized on 1 April 2008 and running through until December 2010, executed on T255 (i.e. approx. 0.7° lon / lat). An example of this evaluation is illustrated in Fig. 1, which shows the evolution of stratospheric O₃ against observations at the Syowa (Antarctica) station. It clearly shows the ability of the C-IFS versions that have stratospheric chemistry to capture the ozone hole, indicating that the stratospheric chemistry within IFS is reasonable. The relatively marginal difference between C-IFS-CB05-BASCOE and C-IFS-Atmos indicates that our approach where tropospheric and stratospheric chemistry are only switched on in troposphere / stratosphere respectively leads to very similar results as a setup where the full reaction schemes for both troposphere and stratosphere are retained throughout the atmosphere (C-IFS-Atmos). A closer look at the gradients at the interface also indicates a smooth interface in photolysis rates between trop and strat. parameterizations (Figure 2), and marginal difference in trace gas profiles between C-IFS-CB05-BASCOE and C-IFS-Atmos. (Figure 3), which gives confidence in

our method. Assessment of trends in O₃ total columns for multi-year simulations suggest in fact that biases are present within C-IFS, but become stabilized after about 1 year simulation time (Figure 4).

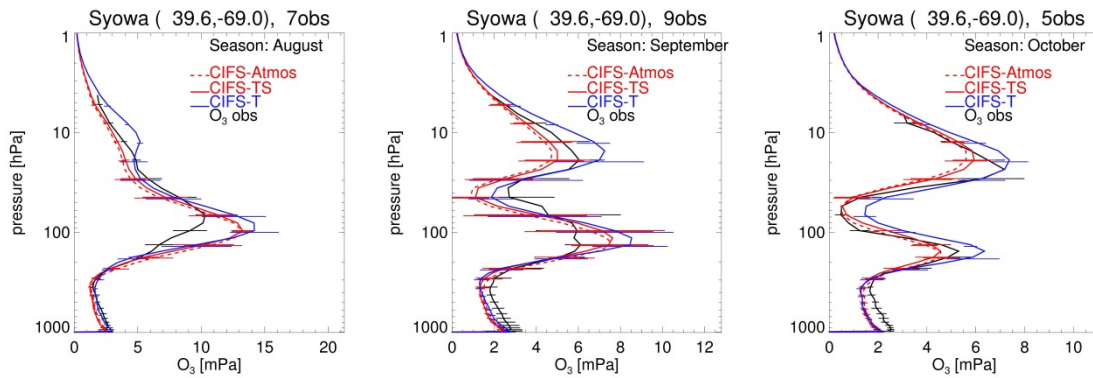


Figure 1. Evaluation of stratospheric ozone against WOUDC ozone sondes at Syowa station during September-November 2009. Black: observations, Red solid: C-IFS-CB05-BASCOE, red dashed: C-IFS-Atmos, blue solid: C-IFS-Cariolle.

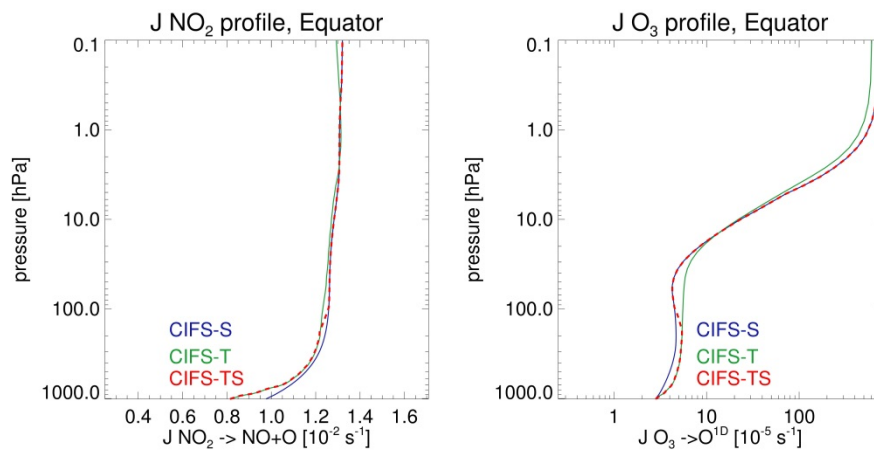


Figure 2. Instantaneous photolysis rates for NO₂ and O₃ at 0°N, 180°W, on 1 October 2008, 0 UTC. Solid blue (CIFS- BASCOE) refers to the stratospheric parameterization, solid green (CIFS-CB05) to tropospheric, and dashed red (C-IFS-CB05-BASCOE) to the merged profile of the rate.

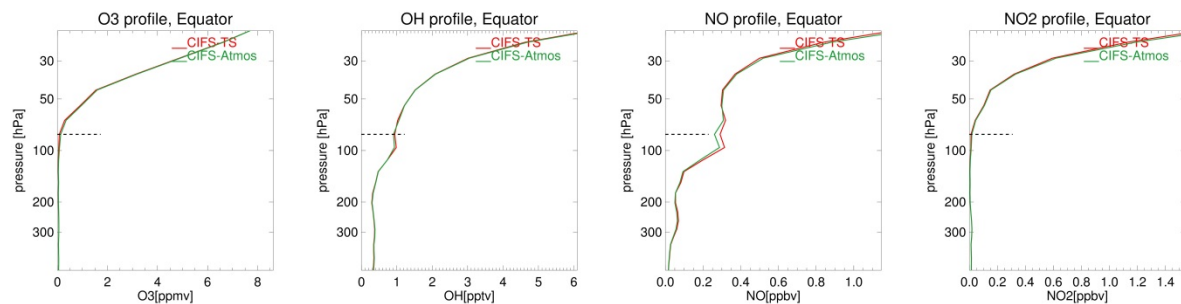


Figure 3. Instantaneous profiles of O₃, OH, NO and NO₂ at 0°N, 180°W, on 1 October 2008, 0 UTC, for runs C-IFS-CB05-BASCOE (red) and C-IFS-Atmos (green). The dashed line denotes the chemical tropopause level associated with the switch in the chemistry mechanism.

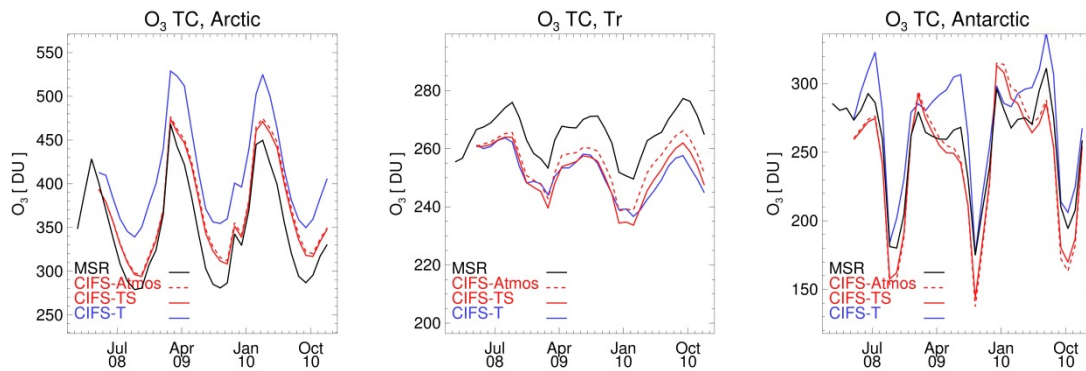


Figure 4. Evaluation of C-IFS-CB05-BASCOE (red, solid), C-IFS-Atmos (red, dashes) and CIFS-Cariolle (blue) monthly mean O_3 total columns in Dobson Units against the Multi-Sensor Reanalysis for the Arctic ($90^{\circ}N-70^{\circ}N$), tropics ($30^{\circ}N-30^{\circ}S$) and Antarctica ($70^{\circ}S-90^{\circ}S$).

Evaluation of current ability of the system for a very large fire event

In response to the large fires over Indonesia during the El Niño drought conditions in September-October 2015, we decided to quickly perform a C-IFS-based study which has been setup quickly where the GFAS fire emissions have been evaluated and optimized in order to estimate the total CO_2 emissions resulting from the peatland fires, to exploit the ability of the system developed within CAMS. Although seasonal fires are a frequent occurrence in the human modified landscapes found in Indonesia, the extent of the 2015 fires was greatly inflated by an extended drought period associated with a strong El Niño. Our methodology is based on a hand-guided inversion methodology for C-IFS simulations of CO, constrained with MOPITT, where we use actually observed in-situ emission ratios of CO_2 and CH_4 to CO. Based on that, we estimated that total carbon released by the fires during Sept-Oct 2015 was 227 ± 67 Tg C, of which 83% is in the form of CO_2 (692 Tg CO_2), 16% CO (84 Tg CO), and 1% CH_4 (3.2 Tg CH_4). We estimate carbon emissions from the 2015 fires to be the largest seen in maritime southeast Asia since those associated with the record breaking El Niño of 1997. Figure 5 shows a map with the spatial distribution of our optimized CO_2 emissions over the region. This study has led to a recent publication (Huijnen et al., 2016b).

Sept-Oct 2015 daily mean CO_2 emissions

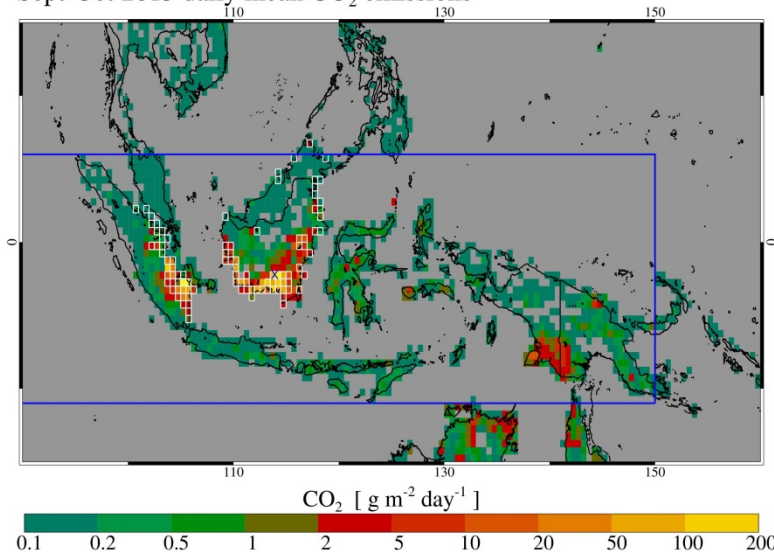


Figure 5. Daily mean CO_2 emissions from peat and vegetation fires burning across maritime southeast Asia in Sept-Oct 2015, presented in $0.5^{\circ} \times 0.5^{\circ}$ grid cells. Cells containing peat soils according to landcover data used in GFASv1.2 are outlined in white.

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.
- 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. Discuss.*, doi:10.5194/gmd-2016-40, in review, 2016a.
- 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, 2016b.
- 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.
- 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)

For the last phase of the current special project we plan to spend work on the optimization of the chemistry solver in terms of numerical efficiency, considering the strong increases in computational costs required for the chemical solver. Work needed for start-up of the CAMS tender on reactive gases is foreseen, in terms of benchmarking and inter-comparing the various branches of C-IFS (MOCAGE and MOZART) as compared to CB05-BASCOE. Also an investigation of the interactions of CIFS-CB05 with the GLOMAP aerosol module, in terms of the chemical precursors, is planned, within the framework of CAMS.