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	2015
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)			700k	533k
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 an improved understanding of the behaviour of stratospheric chemistry in the IFS, and its coupling to the existing tropospheric chemistry based on CB05. Important elements are its current performance in terms of stratospheric ozone, and specifically the ability to capture the ozone hole situation. Also the trends (biases) in long-lived trace gases such as N2O, CFC's, CH4, which tend to develop in simulations exceeding 1 year length are assessed.

At the same time long-term trends in trace gases are assessed that have a short lifetime (NO and NO_2), whose equilibrium concentration depends on the incident solar radiation, but as family (NOx) should be conserved. Furthermore, sensitivity to model resolution in relation to the applied meteorology are assessed. Below these sensitivities are further detailed.

Evaluation of current ability of the system

The performance of C-IFS-BASCOE and C-IFS-CB05-BASCOE has been compared against observations from ozone sondes. For this a run initialized on 1 April 2008 and running through the remainder of the year 2008 was executed on T159 (i.e. approx. 1.1° lon / lat). An example of this evaluation is illustrated in Fig. 1, which shows the evolution of stratospheric O_3 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 functioning. From the figure it can be seen that both implementations show very similar stratospheric O_3, while the C-IFS-BASCOE version, lacking tropospheric chemistry shows a build-up of ozone in the troposphere. Also the evaluation in the troposphere shows reasonable results (see Fig. 2) although the model appears to show a slight negative bias compared to C-IFS-CB05 and observations, specifically in the tropics and over the SH.
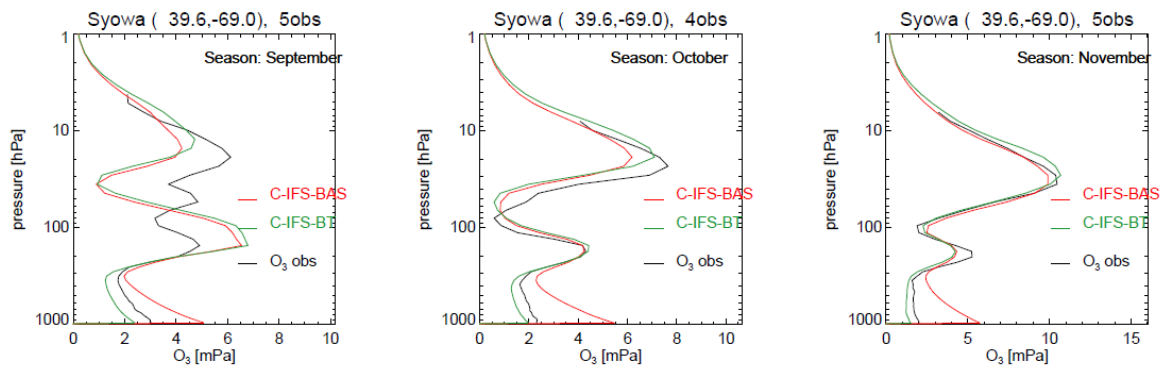
Figure 1. Evaluation of stratospheric ozone against WOUDC ozone sondes at Syowa station during September-November 2008.Black: observations, Red: C-IFS-BASCOE, green: C-IFS-BASCOE-CB05.
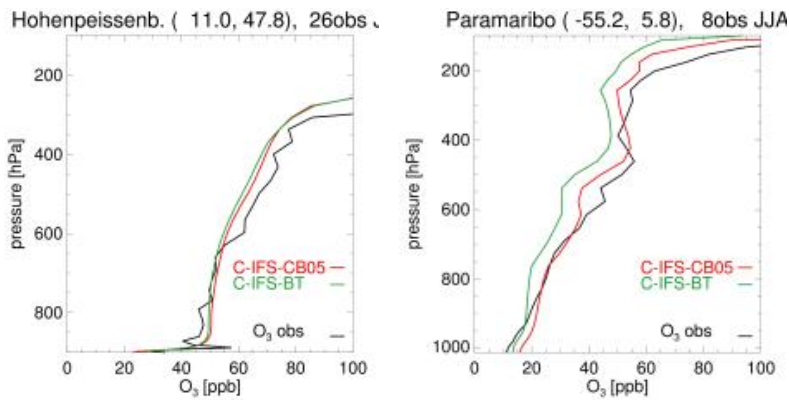

Figure 2. Evaluation of tropospheric ozone against WOUDC ozone sondes at Syowa station during July-August 2008 at Hohenpeissenberg station (left) and Paramaribo station (right). Black: WOUDC, Red: C-IFS-CB05, green: C-IFS-BASCOE-CB05.

Trends in long-lived trace gases

Despite promising results presented in the previous section the model still features significant, unwanted trends in long-lived trace gases as well as, e.g., stratospheric HNO_3. An illustration is given in Fig. 8, showing larger gradients in the N_2O profile over the SH, a significant decline in stratospheric HNO_3, a corresponding decrease in NO_2 and increase in O_3.
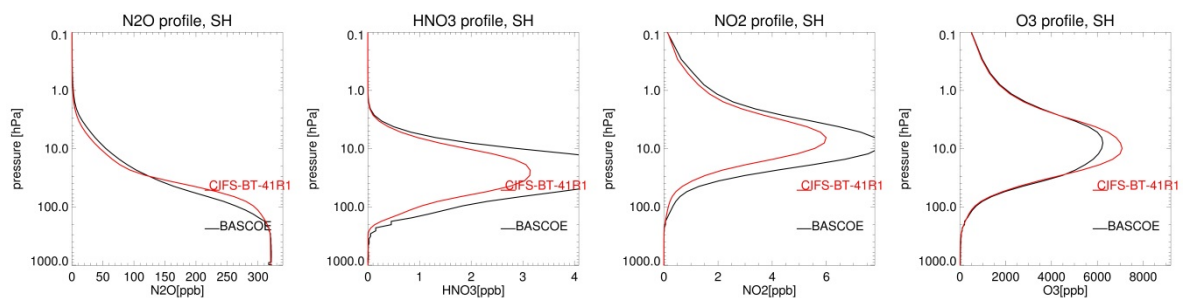

Fig. 3. Evaluation of C-IFS-CB05-BASCOE (red line) zonally averaged trace gas profiles for 1 December 2008, over the extra-tropical SH, as compared to a reference BASCOE offline run (black line).

Specific sensitivity runs have been set up to analyze these biases. In the first sensitivity run the mass of NO, NO_2 and NO_3, which is not conserved as consequence of the semi-Lagrangian advection scheme, is no longer fixed. Compared to the reference run this led to an increase in NO_2 and HNO_3, for 1 October 2008, i.e. after a 1.5 year run, see Fig. 4. As consequence the O_3 has decreased, yielding a much better agreement to the observations.
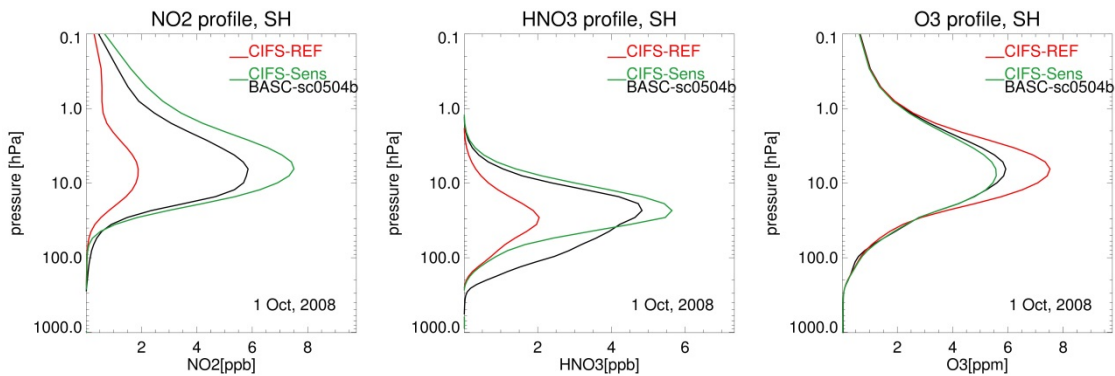
Fig. 4. Evaluation of C-IFS-CB05-BASCOE zonally averaged trace gas profiles for 1 October 2008, over the extra-tropical SH, as compared to a reference BASCOE offline run (black line). In CIFS-REF the mass was fixed after SL-transport for all chemical trace gases, while in run CIFS-Sens the mass fixer for NO, NO_2 and NO_3 was switched off.

An explanation for this contra-intuitive result could be as follows: the NO and NO_2 mass is located near the surface, as consequence of NOx- sources from emissions, and in the stratosphere, related to N_2O break-down. Due to the short-lived nature of the NO and NO_2 tracers, large horizontal gradients related to local surface emissions can be seen. Also there are large gradients at the terminator (sunrise and sunset). These may cause significant local mass budget errors due to the semi-Lagrangian advection. More precisely, the combined tropospheric and stratospheric NO_x showed on average an excess of mass, which needed compensation by decreasing total mass.

By definition a mass fixer scheme cannot a priori differentiate between errors resulting to mass conservation in the troposphere vs those in the stratosphere. In our case, the mass fixer based on the McGregor scheme resulted in a general depletion of the stratospheric NOx. This affected both the HNO_3 and O_3 stratospheric concentrations, see Fig. 4. By switching off the mass firer for NO, NO_2 and NO_3 this problem was largely solved in the stratosphere, where NOx has a relatively long lifetime. At the same time it hardly affected the tropospheric chemistry, as mass budget errors are in this case smaller in magnitude than NOx emissions and therefore do not have a significant impact on the NOx lifetime.

A second test concerned the sensitivity to model resolution. So far most experiments have been executed on a resolution of T159 L60, using a relaxation to ERA-Interim meteorology. We note that this meteorology was generated on T255. As compared to a reference BASCOE simulation a test run with C-IFS on T255 showed a much improved agreement of CH_4, N_2O and CFC's around the tropopause level than a C-IFS run on T159, Figure 5. This illustrated the impact of running on a higher resolution.

The hypothesis is that the relaxation towards a meteorology that had been generated at a different resolution than the one employed for the trace gas experiments results in mismatches of surface pressure field, resulting in spurious pressure waves. While this process is only relevant on relatively large time scales it's effect is not visible on tropospheric chemistry. Still it does affect the mass in the stratosphere, especially the very long-lived trace gases including N_2O and CH_4. This in turn leads to spurious offsets of shorter lived components such as NOx, and hence also stratospheric O_3.
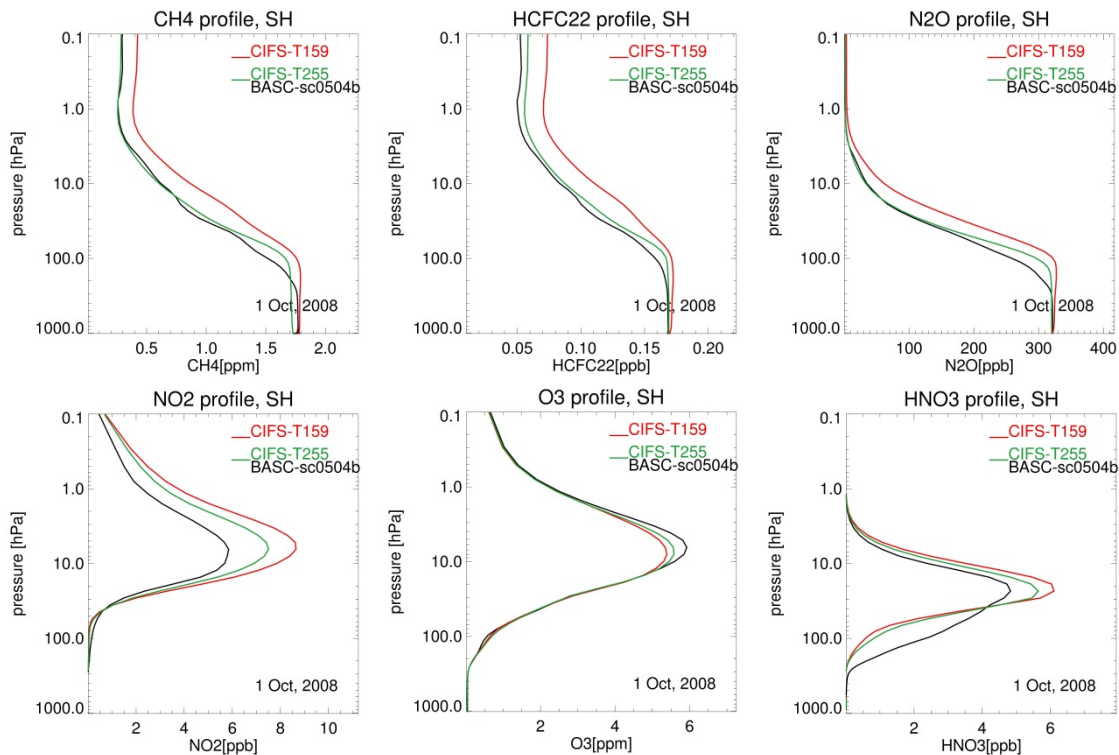
Fig. 5. Evaluation of C-IFS-CB05-BASCOE zonally averaged trace gas profiles for 1 October 2008, over the extra-tropical SH, as compared to a reference BASCOE offline run (black line). In CIFS-T159 uses T159 horizontal resolution while CIFS-T255 uses T255. Profiles are shown for CH4, HCFC22, N2O (top row), NO2, O₃ and HNO₃ (bottom row).

Summary

While tropospheric chemistry based on CIFS-CB05 is relatively well constrained, the extension of the chemistry into the stratosphere still requires substantial effort. Recent investigations showed that switching off the mass fixer for NOx components helps to reduce the negative bias in stratospheric NOx, and therefore reduced the positive bias in O_3. Another finding was that running C-IFS in combination with a relaxation towards ERA-Interim metorology leads to significant drifts in long-lived trace gases such as CH_4 and N_2O, when a different horizontal resolution is used (T159) than the one which was used for ERA-Interim (T255). This implies that any future model studies should be based on a model resolution of (at least) T255, i.e. a significant increase of computational resources will be needed, as compared to what we have foreseen. Finally these findings highlight the sensitive nature of running stratospheric chemistry within the IFS system, as compared to the troposphere.

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

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. Discuss., 8, 1117-1169, doi:10.5194/gmdd-8-1117-2015, 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.

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.

Summary of plans for the continuation of the project

(10 lines max)

For continuation of the project we plan to benchmark the combined tropospheric and stratospheric chemistry in CIFS-CB05-BASCOE. We aim at performing a series of runs with different configurations for the treatment of the stratosphere (linear scheme, full BASCOE chemistry, …)
We furthermore 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.
Also an investigation of the interactions of CIFS-CB05 with the GLOMAP aerosol module, in terms of the chemical precursors, is planned.