# 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** | 2010 |
| **Project Title:** | Global Reactive Gases Modeling in GEMS and MACC: Towards an operational assimilation and forecasting system for tropospheric reactive gases |
| **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:** | 2009 |
| **Expected end date:** | 2011 |

**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) | 100,000 | 60,800 | 100,000 | 108,000 |
| **Data storage capacity** | (Gbytes) | 250 Gb | | 250 Gb | |

## Summary of project objectives
(10 lines max)

The aim of this special project is to facilitate the planned validation work within the final year of GEMS (the first half of 2009), and consecutively use the computational resources in the framework of the MACC G-RG project, for the development, testing and validation of the offline chemistry transport model TM5, the coupled IFS-TM5 system, as well as the novel model system with inline chemistry in IFS (C-IFS). In this framework of this project a reference simulation has been performed with TM5 for the year 2006. Also numerous sensitivity studies with the various model platforms are done to support the development of the C-IFS system.

## Summary of problems encountered (if any)
(20 lines max)

No serious problems have been encountered.

## 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

A detailed evaluation of the tropospheric chemistry transport model TM5 has been finalized (Huijnen et al., 2010). This manuscript contains a description of the various model parameterizations as well as a detailed evaluation of the chemical mechanism compared to a range of observations. This model study serves as a baseline reference for various model developments, including the coupled system created in the GEMS project, as well as the inline chemistry in C-IFS. In the framework of this special project experiments with the offline and coupled IFS-TM5 systems have been facilitated (Elguindi et al., 2010; Flemming et al., 2011).

More recent work focuses on the evaluation of the IFS-TM5 system for the Russian fire period (July-August 2010). For this study several sensitivity runs have been performed, quantifying the effect of the assimilation of atmospheric composition (including IASI CO) and the use of near-real time fire emission estimates from the GFAS system on the forecasting of the chemical composition of the troposphere (Huijnen et al., 2011a).
Fig. 1 shows a time series of CO total columns compared to MOPITT observations. It shows that with the use of the GFAS emissions the model captures very well the increase and decrease of area-averaged CO columns over western Russia. When switching on the assimilation the negative bias is largely resolved, occasionally leading to positive biases during the time of the largest fire emissions. Fig. 1 also shows that for the first forecast day the mean biases are very similar for both runs which use assimilation. But with increasing forecast length the best performance is reached for the configuration that applies both initialization from an analysis and the GFAS emission estimates.

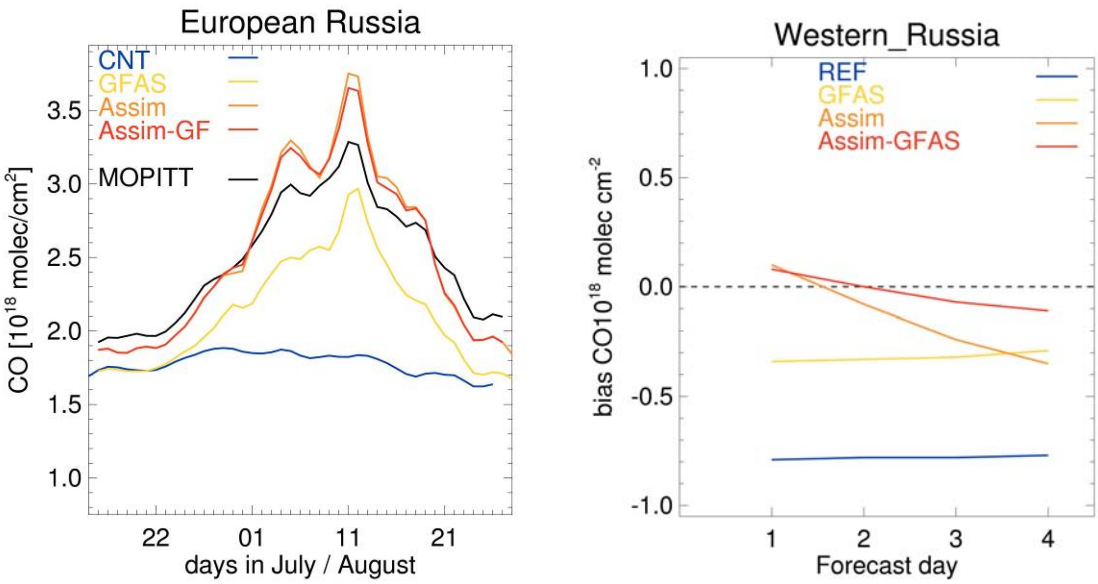


*Figure 1. (left) Evolution of CO total columns over western Russia compared to MOPITT, for $1^{st}$ day forecast results. (right) mean bias as function of forecast day for the period 20 July-15 August.*

Last years computer resources were additionally devoted to the development of the C-IFS inline chemistry scheme, performing series of short and longer sensitivity tests to assess the many parameterizations in this new system as compared to the offline system and observations. Key results are summarized  in the MACC project deliverable G-RG WP 4.7 (Huijnen et al., 2011b). The general findings given in this report are that this version of C-IFS is currently able to produce realistic concentrations with very similar patterns as TM5 of the key trace gases. Absolute differences of C-IFS to TM5 concentration fields are generally in the order of 10-20 %. Yet an overestimation of the oxidative capacity of C-IFS is illustrated by a low bias in CO against MOPITT observations. Also the methane lifetime is only 7.7 year in C-IFS, compared to 8.5 year in TM5. This is consistent with the high bias in tropospheric NO2, which results in too much radical recycling by $NO_x$ as well as an overestimation of ozone production. Fig. 2 shows the zonal mean tropospheric ozone fields for July 2008 in C-IFS and TM5, illustrating the magnitude of the bias. Reasons for the $NO_2$ bias are not yet understood and need further investigation. Such analysis requires a careful evaluation of all chemical and physical processes affecting OH and the NOx cycle. For this purpose additional sensitivity runs have been performed recently, assessing the impact of choices in the photolysis scheme (various cloud optical depth parameterizations), the impact of the stratospheric $NO_x$-treatment, and different options to apply a $NO_x$-family approach. This needs more analysis before clear conclusions can be drawn.

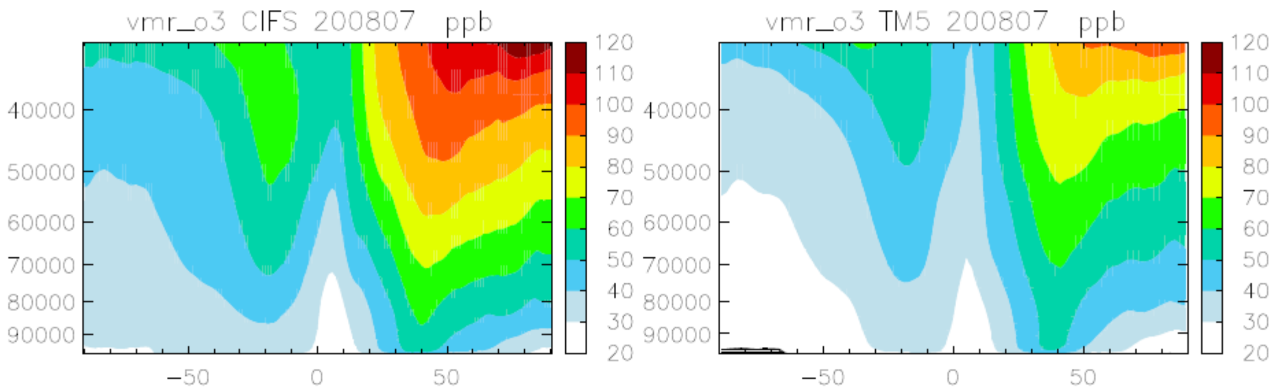


*Figure 2. Zonal monthly mean ozone  concentrations in July  2008 for C-IFS (left) and TM5 (right)*

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

Huijnen, V., Williams, J., van Weele, M., van Noije, T., Krol, M., Dentener, F., Segers, A., Houweling, S., Peters, W., de Laat, J., Boersma, F., Bergamaschi, P., van Velthoven, P., Le Sager, P., Eskes, H., Alkemade, F., Scheele, R., Nédélec, P., and Pätz, H.-W.: The global chemistry transport model TM5: description and evaluation of the tropospheric chemistry version 3.0, Geosci. Model Dev., 3, 445-473, doi:10.5194/gmd-3-445-2010, 2010.

Elguindi, N., Clark, H., Ordóñez, C., Thouret, V., Flemming, J., Stein, O., Huijnen, V., Moinat, P., Inness, A., Peuch, V.-H., Stohl, A., Turquety, S., Athier, G., Cammas, J.-P., and Schultz, M.: Current status of the ability of the GEMS/MACC models to reproduce the tropospheric CO vertical distribution as measured by MOZAIC, Geosci. Model Dev., 3, 501-518, doi:10.5194/gmd-3-501-2010, 2010.

Flemming, J., Inness, A., Jones, L., Eskes, H. J., Huijnen, V., Schultz, M. G., Stein, O., Cariolle, D., Kinnison, D., and Brasseur, G.: Forecasts and assimilation experiments of the Antarctic ozone hole 2008, Atmos. Chem. Phys., 11, 1961-1977, doi:10.5194/acp-11-1961-2011, 2011.

Huijnen, V., Flemming, J. , Kaiser J.W., Inness, A.,  Schultz, M.G., and Heil, A., Assimilation and hindcast experiments of reactive trace gases during the 2010 Russian fires. Proc. Geoph. Res. Abstracts Vol. 13, EGU2011-3169-1, 2011a.

Huijnen, V., Flemming, J., Leitao, J., Bouarar, I., Testing and optimizing of the integrated C-IFS, MACC deliverable report G-RG WP 4.7, 2011b.

## Summary of plans for the continuation of the project

(10 lines max)

The current special project ends this year. As we already used all allocated resources for the current year for the testing of C-IFS, we plan to perform a couple of very short C-IFS sensitivity tests during the remainder of this year based using another budget, and additionally assist in the evaluation of the various model systems using different model runs from colleagues in the project. The focus will be on a detailed assessment of the NOx chemistry and transport in C-IFS, as well on the finalization of the analysis of coupled runs with the TM5-IFS system for the Russian fire case study.