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	2012/13
Project Title:	Global atmospheric chemistry modelling
Computer Project Account:	spdeacm
Principal Investigator(s):	O. Stein, M.G. Schultz
Affiliation:	Research Center Juelich
Name of ECMWF scientist(s) collaborating to the project (if applicable)	J. Flemming, A. Inness, L. Jones, J. Kaiser, R. Engelen
Start date of the project:	2012
Expected end date:	2014

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)	775000	723000	610000	145
Data storage capacity	(Gbytes)	30000	47000	30000	47090

Summary of project objectives

(10 lines max)

- Coupling of the MOZART3 Chemical transport model with the IFS forecast system
- Development of a chemistry module for IFS (C-IFS)
- Evaluation of MOZART3 and the IFS-MOZ coupled model for case study periods defined in the MACC and MACC-II projects including troposphere and stratosphere
- Evaluation of MACC NRT forecasts and reanalysis
- Development of an interoperable web server in Juelich and MACC near-real-time data provision
- investigate global budgets of trace gases in the atmosphere including isotopic composition
- scientific model development of MOZART3 and MOZART-IFS

Summary of problems encountered (if any)

A delay of several months in the development of C-IFS-MOZART in the MACC-II project was experienced due to severe illness of the person in charge of this task.

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

See attached doc-file

List of publications/reports from the project with complete references

- Elguindi, N., Ordóñez, C., Thouret, V., Flemming, J., Stein, O., Huijnen, V., Moinat, P., Inness, A., Peuch, V.-H., Stohl, A., Turquety, S., 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., Flentje, H., Huijnen, V., Moinat, P., Schultz, M. G., and Stein, O.: Coupling global chemistry transport models to ECMWF's integrated forecast system, Geosci. Model Dev., 2, 253-265, 2009.
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- Flemming, J., V. Huijnen, A. Inness, L. Jones, J. Arteta, V.H. Peuch, M.G. Schultz, O. Stein, I. Bouarar, A. Wagner, H. Flentje, J. Leitao, and A. Richter, Atmospheric chemistry in the integrated forecast system of ECMWF, Geophysical Research Abstracts, Vol. 14, EGU2012-9249, 2012
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- Gensch, I., W. Laumer, O. Stein, B. Kammer, T. Hohaus, H. Saathoff, R. Wegener and A. Kiendler-Scharr, Temperature dependence of the kinetic isotope effect in beta-pinene ozonolysis, J. Geophys. Res., 116, D20301, doi:10.1029/2011JD016084, 2011.
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- Inness, A., Baier, F., Benedetti, A., Bouarar, I., Chabrillat, S., Clark, H., Clerbaux, C., Coheur, P., Engelen, R. J., Errera, Q., Flemming, J., George, M., Granier, C., Hadji-Lazaro, J., Huijnen, V., Hurtmans, D., Jones, L., Kaiser, J. W., Kapsomenakis, J., Lefever, K., Leitão, J., Razinger, M., Richter, A., Schultz, M. G., Simmons, A. J., Suttie, M., Stein, O., Thépaut, J.-N., Thouret, V., Vrekoussis, M., Zerefos, C., and the MACC team: The MACC reanalysis: an 8 yr data set of atmospheric composition, Atmos. Chem. Phys., 13, 4073-4109, doi:10.5194/acp-13-4073-2013, 2013.
- Kaiser, J. W., A. Heil, M. O. Andreae, A. Benedetti, N. Chubarova, L. Jones, J.-J. Morcrette, M. Razinger, M. G. Schultz, M. Suttie, and G. R. van der Werf, Biomass burning emissions estimated with a global fire assimilation system based on observed fire radiative power, Biogeosciences, 9, 527-554, doi:10.5194/bg-9-527-2012, 2012.
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- Sahu, S., G. Beig, M. Schultz, N. Parkhi, and O. Stein, Emissions Inventory of Anthropogenic PM2.5 and PM10 in Mega city, Delhi, India for Air Quality Forecasting during CWG- 2010, Geophysical Research Abstracts, Vol. 14, EGU2012-6180, 2012
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- Waychal, S., M. Schultz, M. Decker, S. Lührs, S. Schröder, O. Stein, JOIN: Jülich OWS Interface, Geophysical Research Abstracts, Vol. 15, EGU2013-8949, 2013
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Summary of plans for the continuation of the project

(10 lines max)

Focus for the last year of the project is on the further development of C-IFS and adaptations in the MOZART model which are needed to optimize the chemistry module as well as the deposition and emission modules for C-IFS . More scientifically, global budgets of key trace gases and their interannual variability will be examined and validated using C-IFS, the coupled system IFS-MOZ and MOZART standalone simulations. The Juelich interoperable web services (JOIN) will be further developed to respond flexibly to any changes in the MACC quasi-operational data streams and follow-up products. A continuation of the project after the end of MACC-II in 2014 is foreseen.

Global modelling of atmospheric chemistry
special project SPDEACM interim report
June 2013

Olaf Stein, Martin G. Schultz
Forschungszentrum Jülich

The MOZART global chemistry transport model (CTM) is used in the EU projects MACC and MACC-II as the chemistry module of the coupled MACC weather and chemistry forecast model IFS-MOZ and as one out of three integrated chemistry modules for the C-IFS forecast and assimilation system developed at ECMWF (Stein et al. 2012).

Research conducted with MOZART-3

Beside the successful operation of MOZART-3 in the MACC model system the MOZART standalone chemical transport model is extensively used for process studies and validation purposes. The deficiencies of global Northern Hemisphere CO emissions in the MACC emission inventory MACCity (Granier et al. 2011) and other inventories are tackled in a scientific paper, which is now close to submission (Stein et al. 2013). For this work we performed in total 30 sensitivity studies (1.5 years each) with the MOZART model, 15 of them in the report period (each of one consumed about 45,000 BU and netcdf storage on ECFS of about 400 GB). The Northern Hemisphere wintertime CO underestimation using MACCity was first observed in the MACC reanalysis (Inness et al. 2013) and could be substantiated by using different independent observations. In the reporting period we continued with conducting MOZART offline sensitivity simulations for the year 2008 to test the modelled tracer concentration response to varying emissions. The resulting bias can in principle origin from either an underestimation of CO sources or an overestimation of its sinks. We addressed both the role of sources and sinks and compared our results to observational data from ground-based stations, satellite observations, and MOZAIC tropospheric profiles in close collaboration with MACC colleagues from L'Atmos (Paris), CNRS (Toulouse) and KNMI (De Bilt).

Our MOZART simulation using the MACCity emission inventory underestimated the CO concentrations over the Northern Hemisphere by more than 20 ppb from December to April with a maximal bias of 40 ppb in January (Figure 1, MI). The bias was strongest for the European region but also apparent over North America, implying that wintertime emissions for these regions are missing in the inventory. Such an underestimation is also experienced by other global models (e.g. Shindell et al. 2006). We tested for missing emissions from different sources by facing the model with doubled anthropogenic, biogenic, or biomass burning emissions to the model. For doubled anthropogenic emissions we found an overestimation of CO concentrations all year round although the modelled wintertime concentrations are partly closer to the observation than with the original MACCity emissions. The simulation with doubled biogenic emissions, both from CO and the VOCs, resulted in higher CO concentrations throughout the year, but with a pronounced and unrealistically high maximum during boreal summer. Additionally Southern Hemisphere tropospheric CO was by far overestimated. Similarly, doubling the direct CO emissions from biomass burning, led to a CO overestimation during the main wildfire seasons. This lead to our conclusion that anthropogenic emissions over Europe and North America are missing in the current inventories and that natural emissions do not play a major role for the wintertime bias. Missing anthropogenic VOC emissions would have a small positive impact on the CO concentrations (Figure 1, VOC).

The influence of the dry deposition sink on the global CO budget has been neglected so far by most of the studies on model inter-comparison and source inversion. Although this sink is small compared to the photochemical sink it gains importance during the OH poor winter months. In another sensitivity simulation we exchanged the MOZART CO dry deposition parameterization by

the more advanced scheme from Sanderson et al. (2003), which takes into account the uptake by soils via bacteria and enzymes and is strongly dependant on the soil moisture content. Globally, this parameterization reduced the CO sink by 68 Tg/y with strongest reductions over Europe in wintertime. The resulting Northern Hemisphere surface CO concentrations are enhanced by 20-30 ppb in winter and by 10-15 ppb in summer with largest increase over wintertime Europe (Figure 1, MI-DEP).

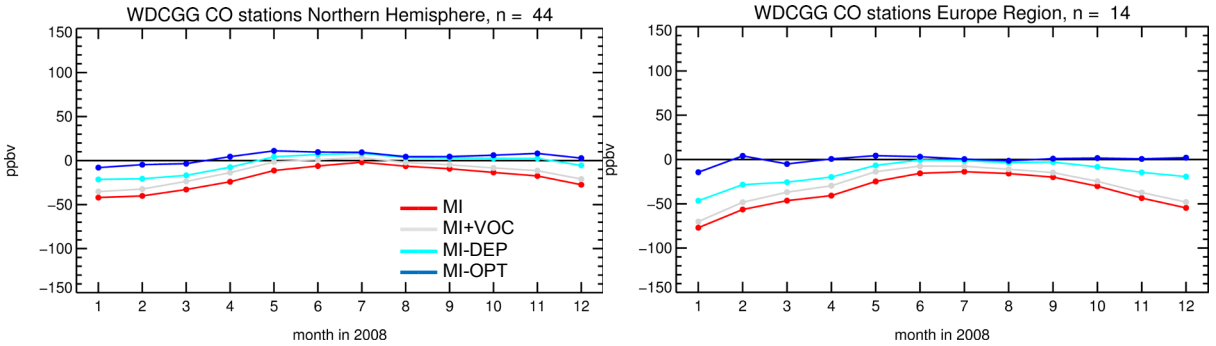

Figure 1: Bias of modelled 2008 monthly mean surface level mixing ratios from the MOZART simulations MI (MACCity), MI+VOC (doubled anthropogenic VOC emissions), MI-DEP (exchanged CO dry dep.), and MI-OPT (optimized sources and sinks) compared to surface observations from WDCGG. n denotes the number of stations used.

To account for the deficits in emissions and deposition, we defined scaling factors for Europen and North American anthropogenic emissions and applied these optimized emissions together with the new dry deposition scheme to the model. The resulting simulation allows to successfully reflect the atmospheric observations (Figure 1 , MI-OPT). In conclusion, the MACCity emission inventory is lacking of anthropogenic emissions over Europe and North America, which could also reflect a wrong seasonality in the inventory or a too optimistic emission reduction in the RCP8.5 scenario used in MACCity.

An updated version of the MEGAN model for biogenic emissions is tested at our MACC partner institute L'Atmos (Paris). Using their latest developments, we applied several MEGAN versions to MOZART in order to facilitate L'Atmos to compare the resulting atmospheric fields to observations. This work is ongoing, a total of about 7 simulations (1.5 years each) will be done by autumn 2013. A scientific paper is in preparation.

In addition the MACC GRG partners started a comparison of stratospheric chemistry schemes for all CTMs employed in the MACC-II project. Initially we compared the photolysis rates in SACADA, BASCOE, and MOZART-3. This work will result in a full intercomparison of stratospheric schemes by the end of 2013 and is lead by partner DLR (Oberpfaffenhofen). For MOZART several shorter simulations (CTM without transport) are planned.

IFS-MOZ

The coupled model IFS-MOZART (Stein et al., 2012) is currently used pre-operationally in the MACC system for NRT production and was also employed in the MACC reanalysis (Inness et al. 2013). Changes related to the MOZART code and to its input data are initiated form this special project. NRT data from the analysis and forecasts (o-suite and e-suite) as well as from the reanalysis and from the GFAS fire emission inventory (Kaiser et al. 2012) are regularly transferred to Forschungszentrum Jülich and made available to the public via our OWS web server JOIN (Schultz et al. 2011). The data transfer from ECMWF is constantly extended to further data, optimized and monitored. The data is also directly accessible to users through the MACC web pages.

C-IFS

Major efforts are ongoing to implement the MOZART3 chemical mechanism into the C-IFS framework. So far MOZART has been adapted for use in C-IFS and input data sets have been prepared. Together with Johannes Flemming (ECMWF) we put together a first version of C-IFS which is able to compile and initially start computation in the ECMWF supercomputer environment. We envisage to complete the technical implementation by the end of 2013, scientifical benchmark tests will be performed until the end of MACC-II. With the expected change to a new supercomputer at ECMWF and the next IFS cycle it will be crucial to extend C-IFS to 91 levels. In principle, the MOZART3 chemistry scheme is prepared to handle chemistry in these extreme altitudes, but several test simulations will be necessary from this special project during the development phase.

In summary, MOZART work is successfully ongoing in the framework of the MACC-II project and the special project is involved for all CTM standalone calculations as well as testing and development of the coupled MACC model and, increasingly important, C-IFS. So far in 2013 not many hpfc resources have been consumed, as some of the model calculations could be done on the Jülich supercomputer. This will change with the upcoming simulations in close cooperation with the MACC-II partners, which can be done at ECMWF only. It is foreseen to apply for a continuation of SPDEACM with a follow-up project beginning in 2015, depending on the post-MACC service development.

References:

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