REQUEST FOR A SPECIAL PROJECT 2013–2015

MEMBER STATE: Germany

Principal Investigator[1]: Olaf Stein

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Project Title:

Global Atmospheric Chemistry Modelling

If this is a continuation of an existing project, please state the computer project account assigned previously.	**SP**DEACM	
Starting year: (Each project will have a well defined duration, up to a maximum of 3 years, agreed at the beginning of the project.)	2012	
Would you accept support for 1 year only, if necessary?	YES ☐	NO X☐

Computer resources required for 2013-2015: (The maximum project duration is 3 years, therefore a continuation project cannot request resources for 2015.)	**2013**	**2014**	**2015**
High Performance Computing Facility (units)	610000	610000	610000
Data storage capacity (total archive volume) (gigabytes)	35000	40000	45000

*An electronic copy of this form **must be sent** via e-mail to:* *special_projects@ecmwf.int*

Electronic copy of the form sent on (please specify date): 2012-04-24

Continue overleaf

[1] The Principal Investigator will act as contact person for this Special Project and, in particular, will be asked to register the project, provide an annual progress report of the project's activities, etc.

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Extended abstract

As already pointed out in the initial description of this special project, we will continue with the integration of gas-phase chemistry from the global chemistry transport model MOZART-3 (Kinnison et al. 2007) into the IFS model for the duration of the EU project MACC-II (2011-2014), which will be one chemistry implementation option for the upcoming C-IFS forecast and assimilation system at ECMWF.

The project work is split into three major parts: First, new model developments and updates in the model input fields will be implemented and tested with the offline model MOZART (version 3.5). Second, the coupled model IFS-MOZART will be further developed and the MACC-II forecasts and reanalysis operated by ECMWF will be supported. Third, the IFS with integrated chemistry (C-IFS) will be developed in close collaboration with ECMWF. Simulations from all three work streams will be validated extensively by FZ Juelich and the MACC-II project partners. In the following the project progress concerning these work packages is described.

MOZART-3

In 2011/2012 the MOZART model used in MACC-II could be further improved, mainly by updates and improvements to the surface boundary fluxes in the model. All model input fields have been revised critically, particularly the deposition fluxes and the emission inventories. For dry deposition, an update of deposition velocity fields has been adapted and tested for MOZART. Dry deposition velocities are also necessary for the development of the C-IFS dry deposition module. For both purposes several MOZART standalone sensitivity simulations have been carried through. A major source of uncertainty still exists within the current emission inventories. As an ongoing work, we investigate the influence of anthropogenic, biogenic, and wildfire emissions on the MOZART model results. It could be shown that the model underestimation of wintertime Northern Hemisphere CO is probably due to missing anthropogenic emission sources of CO and VOCs in the MACCity emission inventory (Granier et al. 2011). First results from this study have been presented at the EGU conference 2012 (Stein et al. 2012a), a scientific paper is in preparation. Other MOZART sensitivity studies focus on alternative biogenic emission estimates for Europe (Steinbrecher et al. 2009) and on the GFAS development in MACC. Recently, the Global Fire Assimilation System, Version1 (GFASv1, Kaiser et al. 2012) has been released by ECMWF. We investigate the MOZART model performance for reactive gases using these and other fire emission estimates (Stein et al. 20012b). All together we conducted 17 standard MOZART3 experiments for the year 2008 up to now each of one consumes about 45,000 BU and netcdf storage on ECFS of about 400 GB. It is foreseen to run another 10 such experiments in 2012/2013.

MOZART simulations with enhanced resolution T106L60 use and estimated computational costs of 270,000 BU per simulation year and netcdf data storage of about 2,400 GB will be run also in 2012/2013, but only for a limited time period, since most of these simulations are done within the IFS-MOZART simulations run by ECMWF. Another comprehensive MOZART simulation (T63L60) will be run in 2012 comprising the years 2003-2012. This simulation will serve the MACC-II project partners for the evaluation of their stratospheric products (DLR) and the NO2 satellite retrievals (U Bremen).

IFS-MOZART

The coupled model IFS-MOZART (Stein et al., 2012c) will be continually employed during MACC-II for the quasi-operational forecasts and a reanalysis. These simulations are operated by ECMWF, but all MOZART related code changes and scripting work will be initiated form this special project. Additional MOZART offline simulations will accompany the ECMWF operations whenever needed.

C-IFS

The integration of modules for chemistry, emissions, and deposition into the IFS module is a major effort of the MACC-II project (Flemming et al. 2012). In the long term this model is intended to take over from IFS-MOZART for operational forecasts of the global chemical state of the atmosphere. MOZART is one out of three chemistry modules initially chosen for C-IFS and is currently being build into the IFS. This major scientific development will continue for the next three years at least. In close collaboration with ECMWF (J. Flemming) the new chemistry module is currently developed based on the existing CTM routines. Experience form related CTMs and GCMs (MOZART-4, ECHAM6-HAMMOZ) will be incorporated into the new chemistry module. This needs extensive testing of the module components both with the C-IFS prototype version and with standalone MOZART simulations. Additionally, the possible usage of the kpp chemistry solver instead of the MOZART solver will be investigated. Another important issue are the optimization of the various interfaces to the aerosol chemistry modules, which are currently not properly defined. Furthermore, the chemistry routines need to be adapted for an extension of C-IFS to a top height of 0.1 hPa. Most of the C-IFS simulations will be operated by ECMWF, but several simulations will be done from this special project during the development phase.

Estimated resources

The yearly estimations (2012-2014) for the simulation runs which are necessary in the MACC-II project have not changed from the original plans and are summarized as follows:

2012

8 years MOZART sensitivity runs in standard resolution T63L60	240000 BU
10 years MOZART long simulation in standard resolution T63L60	300000 BU
2 months MOZART sensitivity runs in enhanced resolution T106L60	45000 BU
Test simulations with the fully coupled chemistry transport model C-IFS	25000 BU

2013/2014

8 years MOZART sensitivity runs in standard resolution T63L60	240000 BU
1 year MOZART sensitivity runs in enhanced resolution T106L60	270000 BU
Simulations with the fully coupled chemistry transport model C-IFS:	100000 BU

Total: 610000 BU and ca. 5000 GB new data storage on ecfs per year

References:

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

Granier, C. et al. (2011), Evolution of anthropogenic and biomass burning emissions of air pollutants at global and regional scales during the 1980–2010 period, Climatic Change, doi:10.1007/s10584-011-0154-1

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.

Kinnison, D. E., Brasseur, G. P., Walters, S., Garcia, R. R.,. Marsh, D. R , Sassi, F., Harvey, V. L., Randall, C. E., Emmons, L., Lamarque, J. F., Hess, P., Orlando, J. J., Tie, X. X., Randel, W., Pan, L. L., Gettelman, A., Granier, C., Diehl, T., Niemeier, U. and Simmons, A. J.: Sensitivity of Chemical Tracers to Meteorological Parameters in the MOZART-3 Chemical Transport Model. J. Geophys. Res, 112, D03303, doi:10.1029/2008JD010739, 2007

Stein, O., M.G. Schultz, I. Bouarar, H. Clark, E. Katragkou, J. Leitao, and A. Heil, Model sensitivity to MACC anthropogenic and biogenic emissions: Global simulations and evaluation for reactive gases, Geophysical Research Abstracts, Vol. 14, EGU2012-7254, 2012a

Stein, O., J.W. Kaiser, A. Heil, and M.G. Schultz, Model sensitivity to global fire emissions: GFED versus GFAS, Geophysical Research Abstracts, Vol. 14, EGU2012-7298, 2012b

Stein, O., J. Flemming, A. Inness, J.W. Kaiser, M.G. Schultz: Global reactive gases and reanalysis in the MACC project, under review at Journal of Integrative Environmental Science, 2012c