REQUEST FOR A SPECIAL PROJECT 2015–2017

MEMBER STATE: Germany

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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.)	2015	
Would you accept support for 1 year only, if necessary?	YES ☐	NO X

Computer resources required for 2015-2017: (The maximum project duration is 3 years, therefore a continuation project cannot request resources for 2017.)	**2015**	**2016**	**2017**
High Performance Computing Facility (units)	750000	600000	600000
Data storage capacity (total archive volume) (gigabytes)	50000	50000	50000

*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): 2014-06-26

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

With the special project SPDEACM will continue our work on development and supervision of the Composition-IFS with MOZART chemistry module (CIFS-MOZ) during the duration of the EU project MACC-III (2014-2015) and beyond for preparation and scientific support of the COPERNICUS atmospheric services operated at ECMWF. Furthermore, the current coupled MACC model for reactive gases IFS-MOZART will be maintained and new CTM developments and updates in the model input fields will be implemented and tested with the offline model MOZART. Simulations from these work streams will be validated extensively by FZ Juelich and the MACC-II project partners. In the following the project progress concerning the work packages is described.

MOZART

Any upcoming updates or improvements in the MOZART chemistry model code will be implemented in the MACC MOZART chemistry (Stein 2013), if relevant for the forecast simulations with CIFS. Similarly, improvements in model input data will be adopted for CIFS. During MACC and MACC-II, several scientific issues have been identified, where further development work is needed for model improvement. This comprises among others the modelled vertical distribution of ozone in the stratosphere (Figure 1; Inness et al. 2013, Lefever et al. 2014), the heterogeneous chemistry on polar stratospheric clouds (PSC; Baier et al. 2014) and the underestimation of Northern Hemisphere wintertime CO due to missing anthropogenic emissions and insufficient dry deposition schemes (Stein et al. 2014). Most of the updates will be integrated directly into CIFS, but model code needs to be prepared to match the IFS conventions and input data needs to be transformed. In contrast to previous projects, all necessary MOZART offline simulations will be done at FZ Jülich, so that no ECMWF CPU resources need to be allocated to this work package, except for data storage on ecfs (about 10 TB/year).

IFS-MOZART

The coupled model IFS-MOZART (Stein et al. 2012) is currently employed as the MACC model for the quasi-operational forecasts and a reanalysis of reactive gases and aerosols. These simulations are operated by ECMWF, but all MOZART related code changes and scripting work will be initiated form this special project. With the switch to the new CRAY supercomputer at ECMWF it is foreseen that IFS-MOZART will be replaced by CIFS. Thus the development and maintenance work done from this special project will be limited.

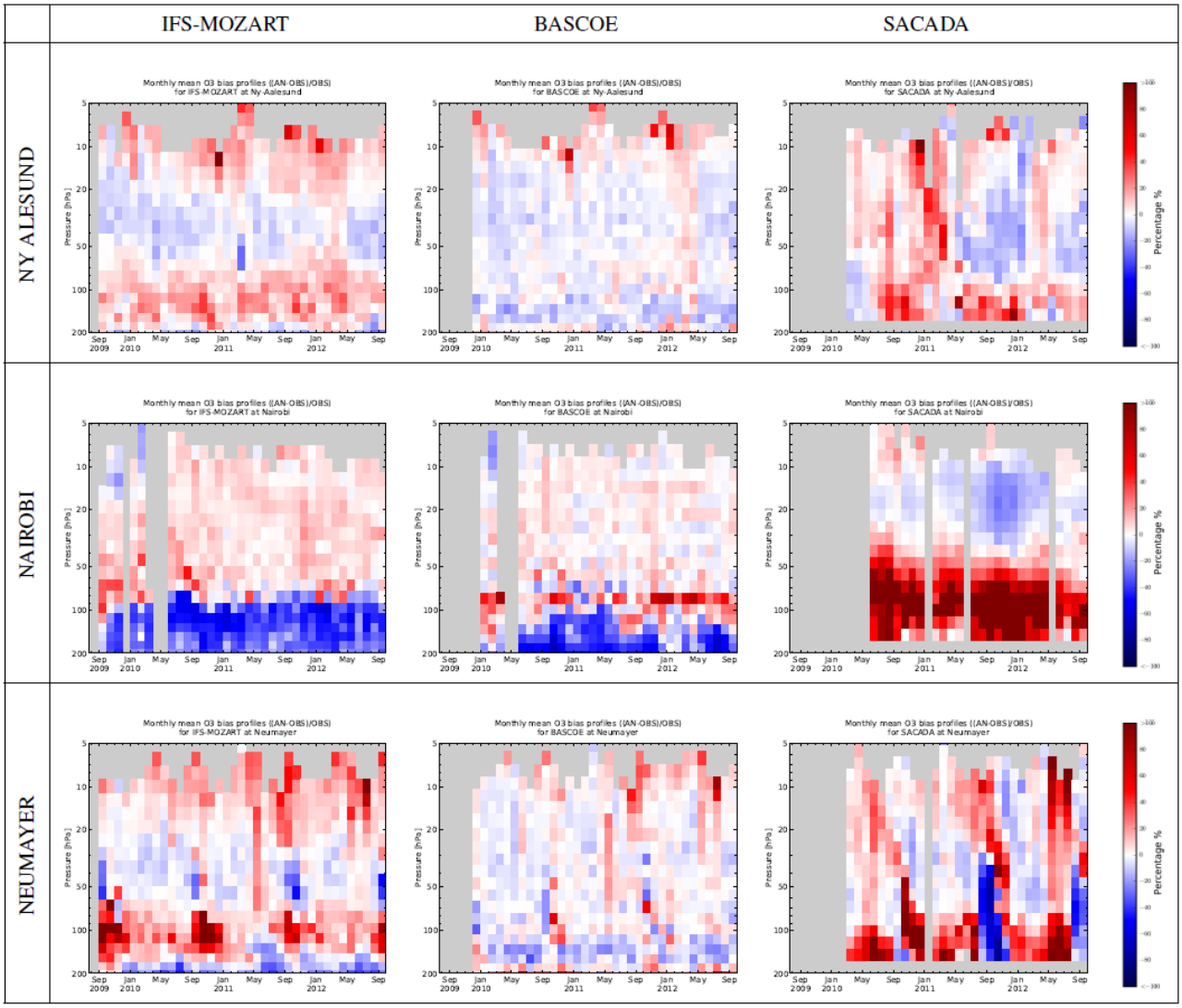

Figure 1: Time series of monthly mean ozone biases (analysis minus observations) with respect to ozone sondes at Ny-A lesund (top panel, 78.92°N, 11.93°E), Nairobi (middle panel, 1.27°S, 36.8°E) and Neumayer (bottom panel, 70.68°S, 8.26°W) for the period September 2009 to September 2012 in %. Left: IFS-MOZART, middle: BASCOE, right: SACADA (adopted from Lefever et al. 2014).

CIFS-MOZ

The MOZART chemistry has been integrated as a chemistry module into the IFS system to build the Composition-IFS (CIFS-MOZ) during MACC and MACC-II (Flemming et al. 2013). CIFS 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 chosen for consideration in CIFS and its implementation is currently tested and evaluated initially. So far a running version of CIFS-MOZ has been successfully tested and short model simulations of 6 days have been completed in the first half of 2014. After fixing a few smaller issues with input data it is envisaged to achieve a first long (~1 year) model simulation in summer 2014. Based on this longer simulation first scientific evaluation of CIFS-MOZ will be performed by FZ Jülich and the MACC-III project partners. Next steps will be the switch to cycle 40R1 and the new CRAY supercomputer. We will also test an updated polar stratospheric cloud calculation as described in Lamarque et al. 2012. With the change to the new supercomputer at ECMWF and the next IFS cycle it will be crucial to extend CIFS 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. Experience form related CTMs and GCMs (MOZART-4,

ECHAM6-HAMMOZ) will be incorporated into the new chemistry module. Additionally, the possible usage of the kpp chemistry solver (Sandu & Sander 2006) 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. In total we plan for 10 simulation years per project year for CIFS-MOZ testing and development. Model output data will be stored on the MARS archive.

JOIN

A task of MACC-III is the continued provision of global boundary conditions for regional air quality modellers world-wide. Near-realtime data from the analysis and forecast simulations (o-suite and e-suite) as well as from the GFAS fire emission inventory (Kaiser et al. 2012) are regularly transferred to FZ Jülich and made available to the public via our OWS web server JOIN (http://join.iek.fz-juelich.de/macc ; Schultz et al. 2011; Waychal et al. 2013). 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. The operation and maintenance of these data streams will be initiated by this special project and is foreseen to continue for the whole project duration.

Estimated resources

The model is currently running under cycle 38R1 with resolution T159L60 (NPES=32, THREADS=8) and takes ~ 10 minutes to run on c2a. It is thus expected that a one-year simulation takes about 10 to 11 hours of computing time or about 50000 BU (very roughly estimated) based on the c2a computer. For T159L91 this number will increase to 75000 BU. The yearly estimations (2015-2017) for the simulation runs which are necessary in the MACC-III project and beyond are summarized as follows (numbers based on c2a):

2015		
	10 years CIFS-MOZ test simulations in resolution T159L91	750000 BU
2016		
	8 years CIFS-MOZ test simulations in resolution T159L91	600000 BU
2017		
	8 years CIFS-MOZ test simulations in resolution T159L91	600000 BU

Total: 1,950,000 BU and ca. 10000 GB new data storage on ecfs per year, some old data can be deleted.

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