SPECIAL PROJECT FINAL REPORT

All the following mandatory information needs to be provided.

Project Title:	Global atmospheric chemistry modelling
Computer Project Account:	spdeacm
Start Year - End Year :	2009 - 2011
Principal Investigator(s)	O. Stein, M. G. Schultz
Affiliation/Address:	Forschungszentrum Jülich GmbH IEK-8: Troposphäre 52425 Jülich Germany
Other Researchers (Name/Affiliation):	S. Schröder, Forschungszentrum Jülich A. Heil, Forschungszentrum Jülich S. Rast, MPI Hamburg

The following should cover the entire project duration.

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 MOZART-IFS model for case study periods defined in the MACC project including troposphere and stratosphere
- Evaluation of MACC NRT forecasts and reanalysis
- investigate global budgets of trace gases in the atmosphere including isotopic composition
- scientific model development of MOZART3 and MOZART-IFS
- development and processing of global emission inventories

Summary of problems encountered

(If you encountered any problems of a more technical nature, please describe them here.)

-

Experience with the Special Project framework

(Please let us know about your experience with administrative aspects like the application procedure, progress reporting etc.)

No problems, flexible responses

Summary of results

(This section should comprise up to 10 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

- Cammas, J.-P., A. Gilles, S. Chabrillat, F. Daerden, N. Elguindi, J. Flemming, H. Flentje, C. Granier, V. Huijnen, A. Inness, L. Jones, E. Katragkou, F. Khokhar, L. Kins, K. Law, K. Lefever, J. Leitao, D. Melas, P. Moinat, C. Ordonez, V.-H. Peuch, G. Reich, M. Schultz, O. Stein, V. Thouret, T. Werner, C. Zerefos, GEMS GRG Comprehensive Validation Report, Toulouse, 2009. http://gems.ecmwf.int/do/get/PublicDocuments/1531/1404
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Future plans

(Please let us know of any imminent plans regarding a continuation of this research activity, in particular if they are linked to another/new Special Project.)

A new special project has been requested in April 2011. The main aim of this special project is the integration of gas-phase chemistry from the global chemistry transport model MOZART-3 into the IFS model, a work which has begun during the EU projects GEMS and MACC and will be continued in the MACC-II project (2012-2014). Continuation of the SPDEACM work is essentially needed after the end of the MACC project in October 2011 in order to ensure the evolution of the MACC system into a fully operational forecast system by 2014. Therefore ECMWF computer resources are foreseen to be continuously needed after October 2011.

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.

Global modelling of atmospheric chemistry
special project SPDEACM final report
June 2011

Olaf Stein, Martin G. Schultz
Forschungszentrum Jülich

The MOZART global Chemical Transport model (CTM) has been used since 2005 in the EU projects GEMS (2005-2009) and MACC (2009-2011), starting as a standalone model with meteorological input data from the IFS, then with the development of the coupled model IFS-MOZART and in parallel as a chemistry module for the IFS with integrated chemistry (C-IFS). IFS-MOZART is an integral part of the global MACC pre-operational reanalysis and forecast system (Flemming et al. 2009) which is foreseen to develop during the successor project MACC-II (2011-2013) into the GMES atmospheric service which will be operational from 2014 on.

In the first two years the MOZART3 CTM has been used for simulations in support of the MACC model developments. Together with the MACC validation partners several peer-reviewed papers on the tropospheric project results could be published: Flemming et al. (2009) describe the coupled system IFS-MOZART as it is used in GEMS and MACC. MOZART modelling results for the European heatwave in summer 2003 are presented in Ordonez et al. (2010). Elguindi et al. (2010) evaluate the ability of the models used in GEMS and MACC to reproduce CO vertical profiles as measured by MOZAIC, while Huijnen et al. (2010) compare the regional and global air quality models (including IFS-MOZART) with regard to OMI NO2 tropospheric columns. Currently another study investigates the statistical evaluation of the MACC reanalysis with CO and NOy MOZAIC flight data in the upper troposphere (Thomas et al. 2011).

For the MACC reanalysis and forecasts a set of new emission inventories have been developed by the project partners. These new emissions consist of the IPCC/MACC anthropogenic emissions which are currently available for the years 2002-2019, updates for natural emissions and wildfire emissions from the new global fire assimilation product (GFAS) available in near-realtime and as a reanalysis from 2003 on.. The new emission inventory data had to be quality-checked and processed for use with MOZART . In the case of wildfire emissions the emission data has been partly produced under the SPDEACM account (Kaiser et al., 2010). MOZART had to be developed to handle the daily resolution of the fire emissions.
The above-mentioned MOZART developments have been implemented also in the coupled model MOZART-IFS, which also had to be prepared carefully for the enhanced MOZART resolution t106 now used in the MACC reanalysis (2003-2010). Also the capability for reading in fire emissions in near-realtime has been developed.

In 2011 several longer sensitivity studies have been carried through to investigate the model sensitivity to the variation of surface boundary conditions. These simulations are currently being extensively validated by the MACC G-RG evaluation partners. It could be shown that the MACC-IPCC emissions provided by D-EMIS (MACCity emission inventory) exhibit too low CO fluxes which in turn leads to an underestimation of tropospheric CO in the model for the Northern Hemisphere. The model results match the observation much better when multiplying the MACC CO traffic emissions by a factor of 2.5, which accounts for a current underestimation of CO traffic emissions under cold engine conditions (Figure 1). The reason for the CO overestimation in the Southern Hemisphere is still unclear. Furthermore strong differences between recent dry deposition fluxes datasets have been found which also lead to differing model results. These investigations are ongoing work in 2011.

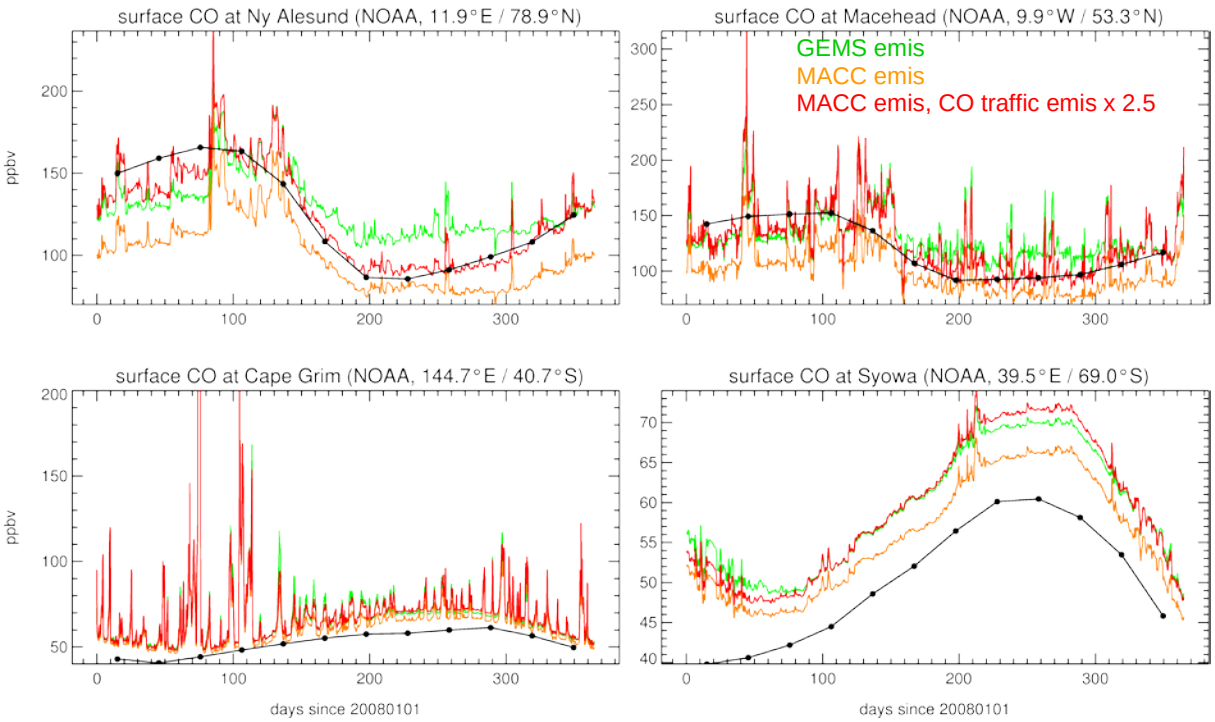

Figure 1: MOZART evaluation with NOAA/GMD station data for 2008 using three different emission data sets. Model data as 3-hourly values, station data as monthly means.

In 2010 and 2011 the MOZART model has been further developed: The problems simulating the right amount of ozone depletion during the Antarctic Ozone hole season has been mostly overcome with the release of a new version of the MOZART3 model (MOZART3.5) in September 2010. This MOZART version supersedes MOZART3.1 (as described in Kinnison et al. 2007) which was up to then employed in the MACC global chemistry simulations. MOZART3.5.02 shows several improvements over previous versions which enhance its capability to adequately simulate Antarctic ozone depletion:

- Updates in the photolysis look-up-table approach
- Local conservation of inorganic chlorine and bromine has been added
- Update of chemical rate constants
- Photolysis extended to solar zenith angles up to 97 degrees
- New sulphate surface area density input files provided from the CCMVal-2 project
- New approach to derive NAT surface area density (variable radius)
- Increased particle numbers from NAT and ice PSCs

A first MOZART3.5 offline simulation for the year 2003 (resolution T63L60) has been performed at FZJ using the NCAR settings for chemistry and emissions but with initial tracer conditions from the MACC reanalysis and meteorological input files from ERA INTERIM. It could be shown from this run that MOZART3.5.02 driven by meteorology from recent IFS versions is able to simulate reasonable stratospheric tracer concentrations and is producing an ozone hole comparable to observations (Figure 2).

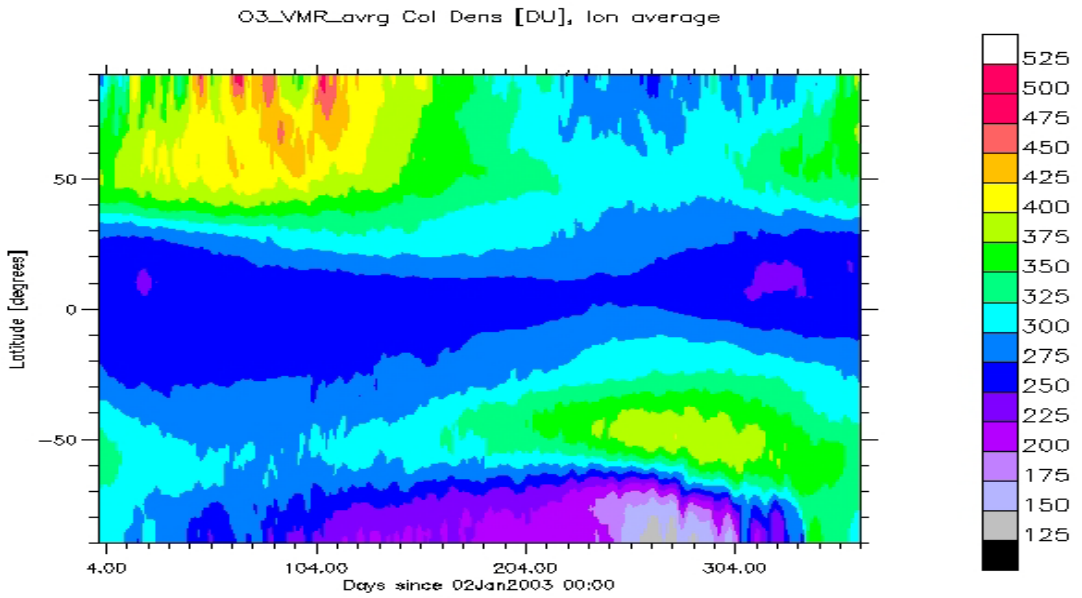

Figure 2: Timeseries of 2003 zonal mean Ozone total column density in Dobson Units as simulated by MOZART3.5.02 with meteorology from ERA-INTERIM and tracer initial conditions from the MACC reanalysis. Minimal total columns are ~136 DU. Note that previous simulations with MOZART 3.1 did not reach values below 200 DU.

After successful initial testing, the code modifications and extensions which had been developed in GEMS and MACC were re-introduced into the MOZART3.5.02 code. This updated MACC MOZART offline model was delivered to ECMWF in October 2010. Major code modifications include:

- Use of MACC fire emission inventory in daily resolution
- Use of MACC anthropogenic and natural emission inventories
- Integration of SOx and NH3 chemistry routines from MOZART4 (Emmons et al. 2010)

A first offline simulation with the complete MACC settings yields results that are fairly similar to the run with NCAR settings (Figures 3 and 4). In the meantime the new code version is also integrated in the IFS-MOZART model code and ready for use in cycle 37r3.

The new model serves as a basis for the integrated MACC chemistry model MOZART-IFS as well as for the C-IFS developments and it will be used for offline CTM comparisons. In the meantime the new code version is also integrated in the coupled setup for the quasi-operational MACC system and ready for use in cycle 37r3. A paper has been published recently showing the stratospheric performance of the coupled model IFS-MOZART (Flemming et al. 2011).

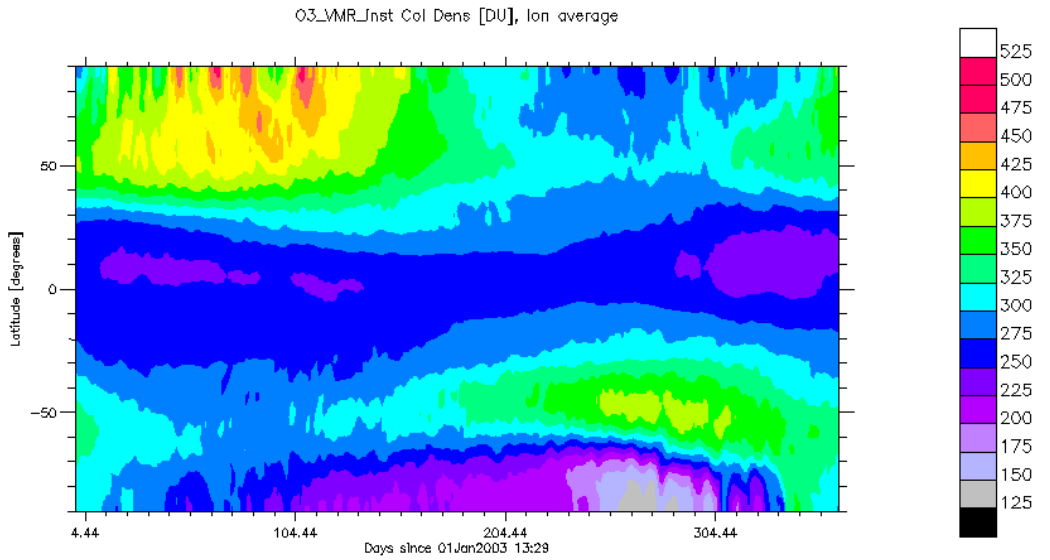

Figure 3: As Figure 2, but using MACC initial fields and boundary conditions

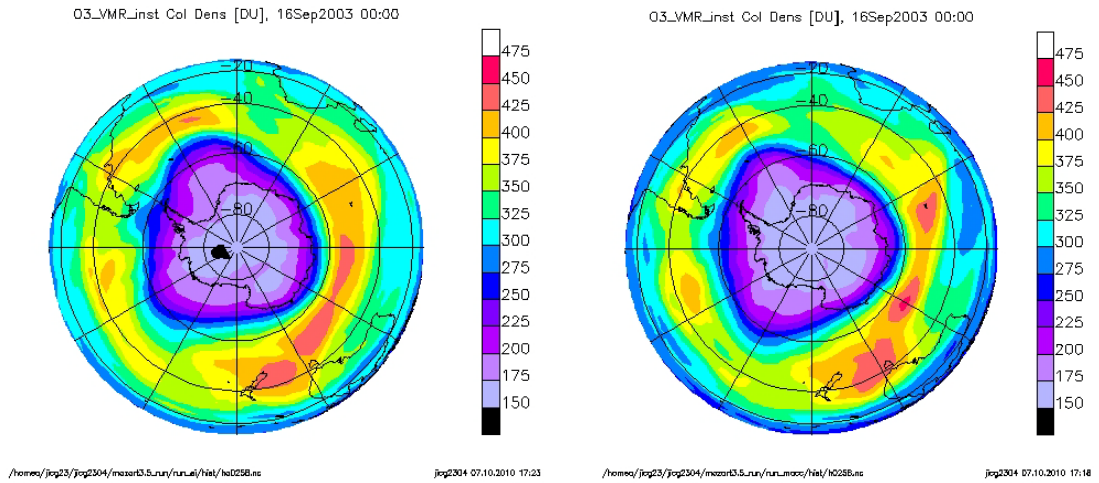

Figure 4: Comparison between a MOZART 3.5 simulation with NCAR settings (left) and MACC settings (right) for 16 September 2003. The small differences are most likely due to the different initial conditions used

An important service from the global MACC component is the provision of chemical boundary conditions for regional air quality (RAQ) models. This service has been extended considerably in the last three years. Originally boundary conditions have been provided for the European RAQ models in the GEMS project only. Since June 2010 we are able to offer the aerosol and gas-phase tracer boundary conditions for other regional modellers worldwide via a WCS server installed at Forschungszentrum Jülich (http://macc.icg.kfa-juelich.de:50080/). Data is transferred from the MARS and ECFS archives and is available only hours after the completion of the MACC forecast. Data can be compared with observational station data which is currently available only for Germany (Figure 5). Since May 2011 near-realtime fire emissions from the global fire assimilation system (GFAS) developed at ECMWF are also available from the server.

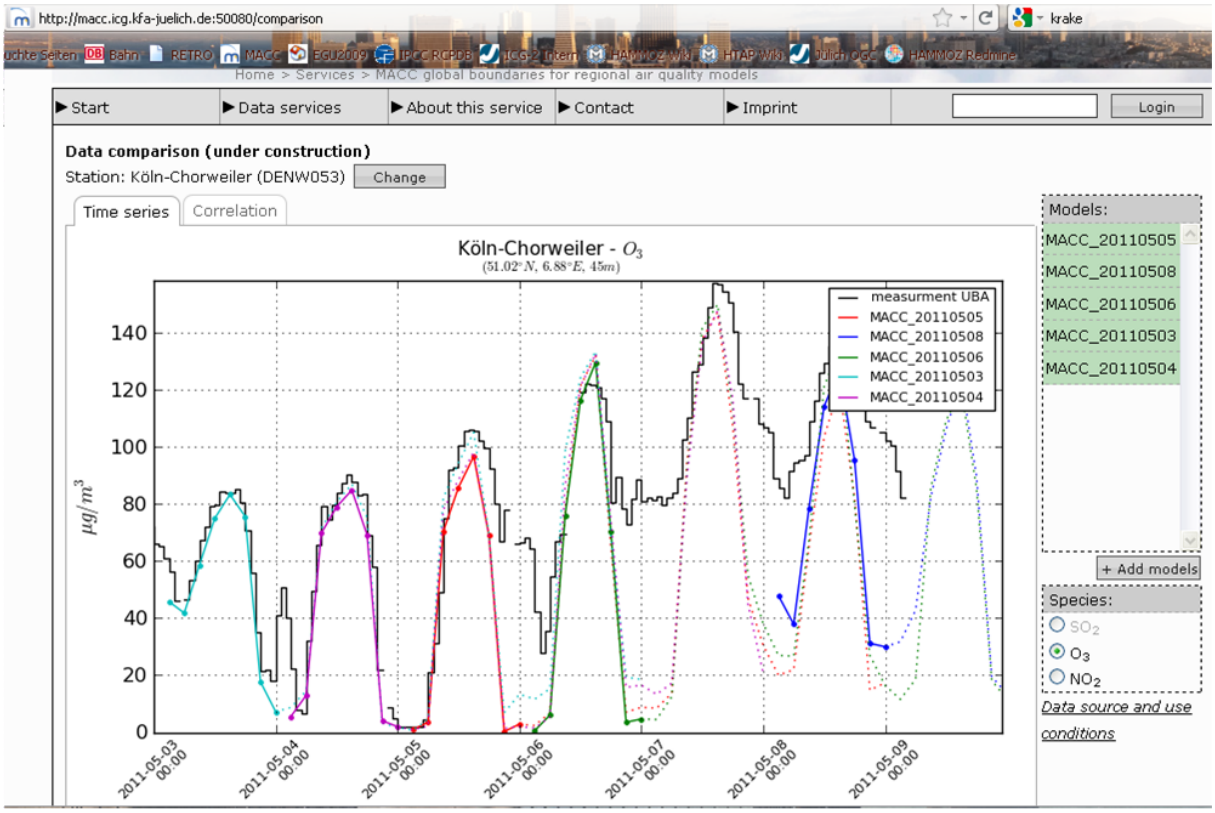

Figure 5: Snapshot from Jülich WCS server: MACC ozone forecasts interpolated to the station Köln-Chorweiler for the period 2011-05-03 to 2011-05-09 compared to station observations (available from Umweltbundesamt, Germany) . Daily forecasts are displayed as straight lines, observations for days 2-4 as dotted lines.

In addition to the MACC activities modelling of stable carbon isotopes of volatile organic compounds (VOC) is ongoing. A paper on stable carbon isotope ratios of ethane over the North Pacific could be published (Saito et al., 2011), another study dealing with the temperature dependence of the kinetic isotope effect in peta-pinene ozonolysis has been submitted to JGR (Gensch et al. 2011). For these studies existing MOZART standalone model simulations from the GEMS and MACC projects could be used.

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