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	2014/15
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, R. Engelen
Start date of the project:	2014
Expected end date:	2017

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)	610000	31837	750000	395852
Data storage capacity	(Gbytes)	30000	47570	30000	47737

Summary of project objectives

(10 lines max)
- Development of a chemistry module for IFS (CIFS-MOZ)
- Maintenance and improvements of the quasi-operational coupled MACC system MOZ-IFS
- Evaluation of the MOZ-IFS and CIFS-MOZ model for the troposphere and stratosphere
- Evaluation of MACC NRT forecasts and reanalysis
- investigate global budgets of trace gases in the atmosphere
- scientific model development of gas-phase chemistry in MOZART3, MOZ-IFS and CIFS-MOZ
- development and processing of global emission inventories

Summary of problems encountered (if any)

Due to change of contract of O. Stein at FZ Jülich and end of the MACC project the model simulations within spdeacm during the year 2014 needed to be restricted to a minimum. This has been changed again in 2015 with the start of Yi Heng as new group member.

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

Peer-reviewed:

Eskes, H., Huijnen, V., Arola, A., Benedictow, A., Blechschmidt, A.-M., Botek, E., Boucher, O., Bouarar, I., Chabrillat, S., Cuevas, E., Engelen, R., Flentje, H., Gaudel, A., Griesfeller, J., Jones, L., Kapsomenakis, J., Katragkou, E., Kinne, S., Langerock, B., Razinger, M., Richter, A., Schultz, M., Schulz, M., Sudarchikova, N., Thouret, V., Vrekoussis, M., Wagner, A., and Zerefos, C.: Validation of reactive gases and aerosols in the MACC global analysis and forecast system, Geosci. Model Dev. Discuss., 8, 1117-1169, doi:10.5194/gmdd-8-1117-2015, 2015.

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Gaudel, A., H. Clark, V. Thouret, L. Jones, A. Inness, J. Flemming, O. Stein, V. Huijnen, H. Eskes, P. Nedelec, D. Boulanger: On the use of MOZAIC-IAGOS data to assess the ability of the MACC Reanalysis to reproduce the distribution of O3 and CO in the UTLS, submitted to TELLUS B, 2015.

Inness, A., Blechschmidt, A.-M., Bouarar, I., Chabrillat, S., Crepulja, M., Engelen, R. J., Eskes, H., Flemming, J., Gaudel, A., Hendrick, F., Huijnen, V., Jones, L., Kapsomenakis, J., Katragkou, E., Keppens, A., Langerock, B., de Mazière, M., Melas, D., Parrington, M., Peuch, V. H., Razinger, M., Richter, A., Schultz, M. G., Suttie, M., Thouret, V., Vrekoussis, M., Wagner, A., and Zerefos, C.: Data assimilation of satellite-retrieved ozone, carbon monoxide and nitrogen dioxide with ECMWF's Composition-IFS, Atmos. Chem. Phys., 15, 5275-5303, doi:10.5194/acp-15-5275-2015, 2015.

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Kracher, D., C. Reick, E. Manzini, M. G. Schultz, O. Stein, Global warming reduces climatic impact of N2O by an accelerated Brewer-Dobson circulation, submitted to Nature Climate Change, 2015.

Lefever, K., van der A, R., Baier, F., Christophe, Y., Errera, Q., Eskes, H., Flemming, J., Inness, A., Jones, L., Lambert, J.-C., Langerock, B., Schultz, M. G., Stein, O., Wagner, A., and Chabrillat, S.: Copernicus stratospheric ozone service, 2009–2012: validation, system intercomparison and roles of input data sets, Atmos. Chem. Phys., 15, 2269-2293, doi:10.5194/acp-15-2269-2015, 2015.

Sheel, V., L. K. Sahu, M. Kajino, M. Deushi, O. Stein, P. Nedelec, Seasonal and inter-annual variability of carbon monoxide based on MOZAIC observations, MACC reanalysis and model simulations over an urban site in India, J. Geophys. Res. Atmos., 119, 9123–9141, doi:10.1002/2013JD021425, 2014.

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Wagner, A., Blechschmidt, A.-M., Bouarar, I., Brunke, E.-G., Clerbaux, C., Cupeiro, M., Cristofanelli, P., Eskes, H., Flemming, J., Flentje, H., George, M., Gilge, S., Hilboll, A., Inness, A., Kapsomenakis, J., Richter, A., Ries, L., Spangl, W., Stein, O., Weller, R., and Zerefos, C.: Evaluation of the MACC operational forecast system – potential and challenges of global near-real-time modelling with respect to reactive gases in the troposphere, Atmos. Chem. Phys. Discuss., 15, 6277-6335, doi:10.5194/acpd-15-6277-2015, 2015.

Other publications:

Baier, F., S. Chabrillat, and O. Stein, Report on differences in stratospheric chemistry schemes and their potential impact on model results, MACC-II Deliverable D_57.2, April 2014. https://www.gmes-atmosphere.eu/documents/maccii/deliverables/grg/MACCII_GRG_DEL_D57.2_May2014.pdf

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Kaiser, J. W., N. Andela, J. Atherton, M. de Jong, A. Heil, R. Paugam, S. Remy, M. G. Schultz, G. R. van der Werf, T. T. van Leeuwen, M. J. Wooster, Recommended fire emission service enhancements, Technical Memorandum, 724, Reading, May 2014. http://old.ecmwf.int/publications/library/ecpublications/_pdf/tm/701-800/tm724.pdf

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Kracher, D., Manzini, E., Schultz, M., Stein, O., Reick, C. H., Distribution of N2O in the atmosphere under global warming – a simulation study with the MPI Earth System Model, Geophysical Research Abstracts, Vol. 16, EGU2014-5777, 2014.

Rudolph, J. and O. Stein, Tropospheric Chemistry and Composition, Aliphatic Hydrocarbons, in: Encyclopedia of Atmospheric Sciences, 2nd ed., vol. 6, pp. 188-203, ISBN 978-0-12-382225-3, doi:10.1016/B978-0-12-382225-3.00423-0, 2015. http://www.sciencedirect.com/science/article/pii/B9780123822253004230

Stein, O. and J. Flemming, Documentation of C-IFS-MOZ, MACC-III Deliverable D_24.4, April 2015.

Tsikerdekis, A., E. Katragkou, P. Zanis, D. Melas, H. J. Eskes, J. Flemming, V. Huijnen, A. Inness, I. Kapsomenakis, M. Schultz, O. Stein, C. Zerefos: Comparison between assimilated and non-assimilated experiments of the MACCii global reanalysis near surface ozone, Geophysical Research Abstracts, Vol. 16, EGU2014-652, 2014.

For any publications prior to 2014 we refer to the references in the spdeacm final report 2012-2014.

Summary of plans for the continuation of the project

(10 lines max)

Currently spdeacm is supporting scientific work which is in a transition phase between the European project MACC-III and the upcoming CAMS prpoject led by ECMWF. It is planned for 2015-2017 to continue the development of CIFS-MOZ and to bring this model to an operational state. Moreover, 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.

Global modelling of atmospheric chemistry special project SPDEACM interim report

June 2015

Olaf Stein, Martin G. Schultz
Forschungszentrum Jülich

In 2014/2015 the global model system CIFS-MOZ (IFS with integrated MOZART chemistry) has been further developed such that there is now a stable and reliable version ready for use in scientific applications. The coupled MACC system IFS-MOZ (Stein et al., 2012) was used for the quasi-operational analyses and forecasts until September 2014. The scientific project is now in a transition phase between MACC-III and CAMS led by ECMWF. Due to change of contract of O. Stein at FZ Jülich and end of the MACC project the model simulations within spdeacm during the year 2014 needed to be restricted to a minimum. This has been changed again in 2015 with the start of Yi Heng as new group member. A series of peer-reviewed papers could be published or are submitted from the MACC project with spdeacm participation.

C-IFS

After installing the MOZART interface in CIFS in 2014 we successfully conducted longer simulations (~1 year) on cca. The first model runs were initially evaluated against observations and other CIFS implementations CIFS-CB05 and CIFS-MOCAGE (Flemming et al., 2014). Starting in 2015, the latest version of CIFS-MOZ was updated to IFS cycle 41R1 on the new CRAY machine (cca). Due to the substantial changes in the IFS model and scripts together with our limited capacities we needed about three months to establish a stable version of CIFS-MOZ on cca. The model is now ready for scientific applications and a first sensitivity test was conducted where the global mass fixer for NOx species has been switched off (Fig. 1).

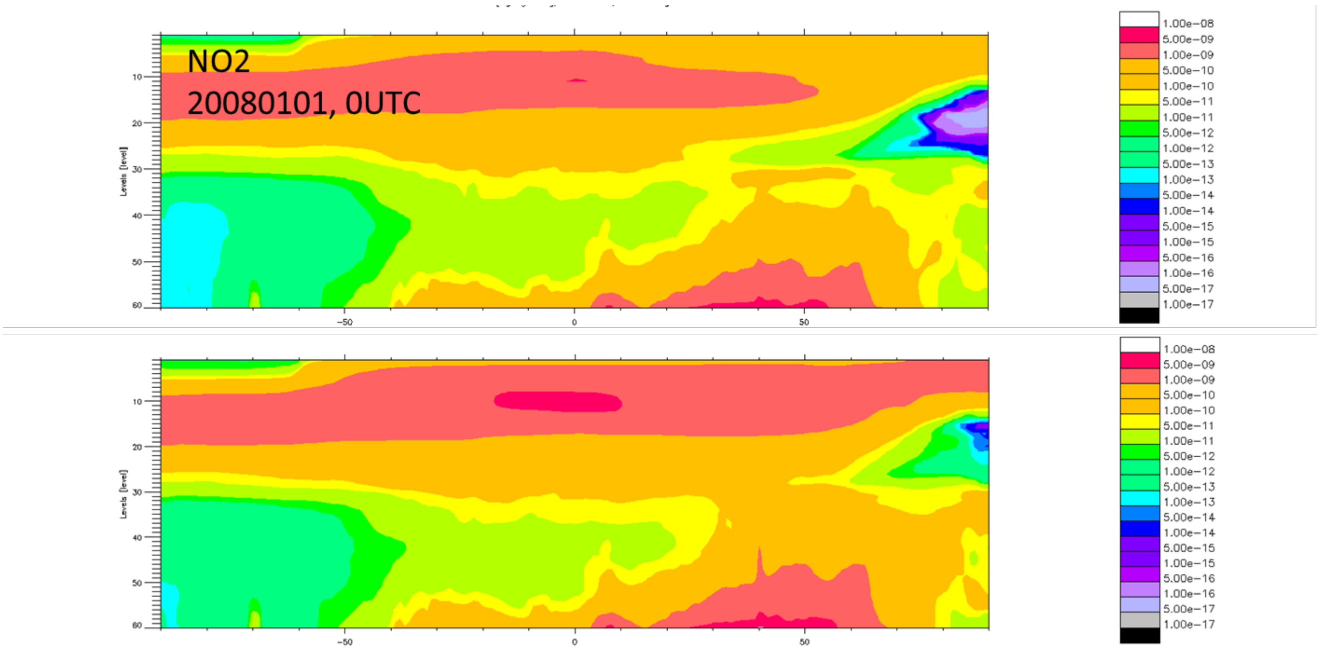

Fig. 1: NO2 zonal mean mass mixing ratios [kg kg-1] at 20080101, 0 UTC from a CIFS-MOZ simulation with (top) and without (bottom) global mass fixer for NOx species

For our applications CIFS-MOZ is currently running with resolution T255L60 (NPES=48, THREADS=4). Costs are about 200000 BU per model year with this resolution. It needs to be defined finally, which resolution is needed for comparison model simulations. Partly model runs with CIFS-MOZ can also be done directly from ECMWF accounts. Depending on these decisions on simulation set-ups we may need to apply for additional HPC resources for the coming years. The actual CIFS-MOZ implementation is described in detail in Stein et al. (2015).

SPDEACM also contributed to the current pre-operational MACC-III version of CIFS, namely CIFS-CB05 (Flemming et al., 2015). We supported the development of CIFS-CB05 by defining input data, comparing and updating chemistry schemes and harmonizing the chemistry tables for the different CIFS implementations. Of particular interest is the integration of BASCOE stratospheric chemistry into CIFS-CB05 which needs to be compared to the existing full atmospheric schemes available with MOZART or MOCAGE CTMs (Fig. 2). For this purpose we will introduce in 2015 an updated scheme for polar stratospheric clouds in CIFS-MOZ.

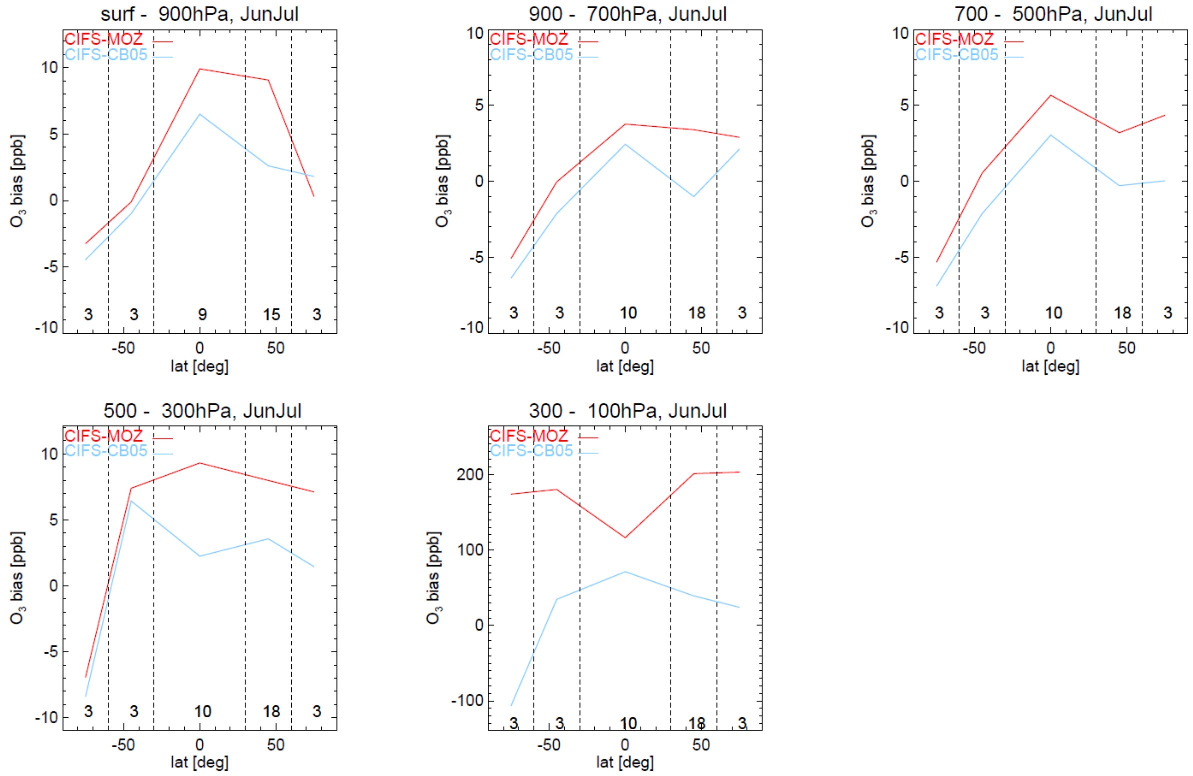

Figure 2: Mean model bias of CIFS-MOZ and CIFS-CB05 against ozone sondes at April 1, 2008 at various latitude and altitude ranges. The number in each latitude range indicate the amount of stations that contribute to the statistics.

NRT data from the MACC 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 interface JOIN (Waychal et al. 2013). JOIN (http://join.iek.fz-juelich.de/) provides a user friendly interface for flexible selection of data sets delivered from WCS servers. The user can select a geographical region, time range and different variables from the selected dataset and then can download or visualize the data in the form of maps, vertical cross sections or time series. JOIN uses standards like WCS, CF-netCDF and INSPIRE to test in a real-life environment.

IFS-MOZ

The coupled MACC system IFS-MOZ has been running quasi-operationally at ECMWF from 2010 to September 2014 for the MACC forecasts and analyses. Additionally it was used for the MACC reanalysis (2003-2012). In October 2014 this system was superseded by the first version of CIFS. During the last year, several scientific papers discussed and evaluated these simulations.

Lefever et al. (2015) address the quality of the stratospheric ozone analyses between September 2009 and September 2012. The MOZART-IFS chemical data assimilation system is compared to the Belgian Assimilation System for Chemical ObsErvations (BASCOE), the Synoptic Analysis of Chemical Constituents by Advanced Data Assimilation (SACADA), and the Data Assimilation Model based on Transport Model version 3 (TM3DAM). The MACC system delivered total column values that agree well with ground-based observations (biases < 5%) and have a realistic seasonal cycle. Vertically alternating positive and negative biases are found in the MOZART-IFS analyses as well as an overestimation of 30 to 60% in the polar lower stratosphere during polar ozone depletion events (Fig. 3).

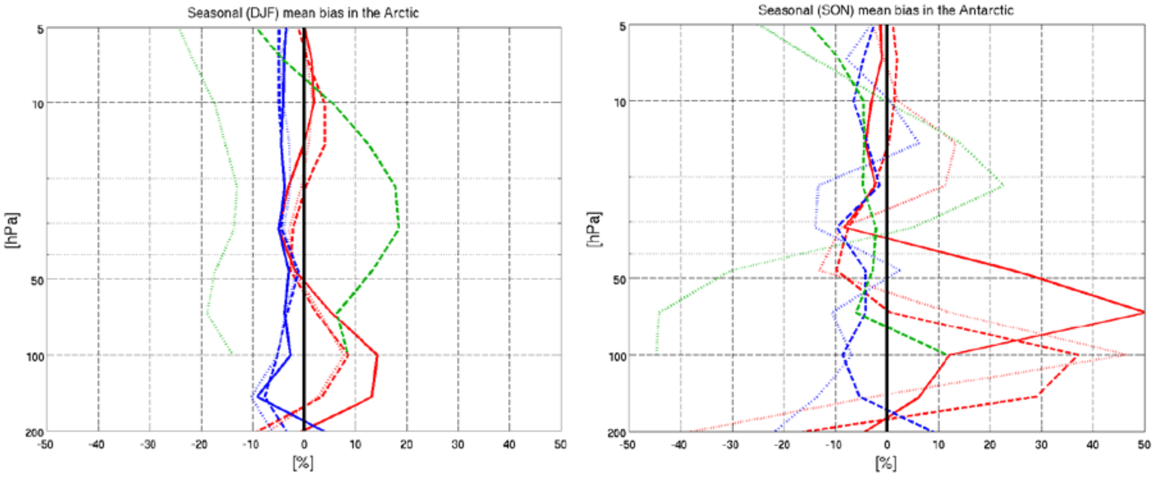

Figure 3: Seasonally averaged relative ozone bias profiles of IFS-MOZART (red), BASCOE (blue), and SACADA (green) versus ACE-FTS (AN minus OBS) in % for the Arctic winter (DJF) 2009-2010 (full), 2010-2011 (dashed), 2011-2012 (dotted) and the Antarctic spring (SON) 2009 (full), 2010 (dashed), and 2011 (dotted).

Reactive gases (O_3, CO, NO_2) in the troposphere from the MACC system are evaluated by Wagner et al. (2015). The validation was performed based on CO and O_3 surface observations from the Global Atmosphere Watch (GAW) network, O_3 surface observations from the European Monitoring and Evaluation Programme (EMEP), NO_2 tropospheric columns derived from the satellite sensors SCIAMACHY and GOME-2, and CO total columns derived from MOPITT. The MACC system proved capable of reproducing reactive gas concentrations in consistent quality, however, with some seasonally dependent bias compared to surface and satellite observations.

The MACC reanalysis (Inness et al., 2013) has gained a widespread attention. SPDEACM contributed directly to three papers: Sheel et al. (2014) compared MACC reanalysis results for CO profiles over an urban site in India with MOZAIC aircraft profiles and other model calculations. They showed that mean biases with respect to the observed CO profiles were lower for the MACC reanalysis than for model simulations with MOZART and MRI-CCM2. The CO in the PBL region was consistently underestimated by MACC reanalysis during all the seasons, while the other models show both positive and negative biases depending on the season.

Katragkou et al. (2015) evaluate the MACC reanalysis with respect to near surface ozone for specific European subregions. Measurements at rural locations from the European Monitoring and Evaluation Program (EMEP) and the European Air Quality Database (AirBase) are used for this evaluation assessment. The annual overall error of near surface ozone reanalysis is on average 24% over Europe, the highest found over Scandinavia (27%) and the lowest over the Mediterranean marine stations (21%). Near surface ozone shows mostly a negative bias in winter and a positive bias during warm months. Assimilation reduces the bias in near surface ozone and its impact is mostly notable in winter. With respect to the seasonal cycle, the MACC reanalysis reproduces the photochemically driven broad spring-summer maximum of surface ozone of central and south Europe. However, it does not capture adequately the early spring peak and the shape of the seasonality at northern and north-eastern Europe.

The performance of the MACC reanalysis and a control run without data assimilation in the extratropical upper troposphere/lower stratosphere (UTLS) over Europe is assessed in Gaudel et al. (2015) with MOZAIC/IAGOS in-flight data for ozone and CO. On average over the period, the reanalysis underestimates O3 by 60 ppbv in the lower stratosphere (LS), whilst CO is overestimated by 20 ppbv. In the upper troposphere (UT), O3 is overestimated by 50 ppbv, but CO is partly over or underestimated by up to 20 ppbv. As expected, assimilation generally improves model results.

Research conducted with MOZART-3 (off-line model)

The offline-CTM MOZART-3 driven by ECMWF dynamics is an effective tool to test the model sensitivity to changing initial or boundary conditions or to other changes in the model chemistry. In 2014 we published a paper on the wintertime low bias of northern hemisphere CO in global model studies, which has been summarized already in the last spdeacm interim report (Stein et al., 2014). In this work also a detailed atmospheric budget of CO is given based on model calculations performed within spdeacm (Fig. 4). Adding to earlier work on volatile organic compounds (VOC), the book chapter in “Encyclopedia of Atmospheric Sciences” summarizes current knowledge about aliphatic hydrocarbons, including results from MOZART model calculations (Rudolph and Stein, 2015).

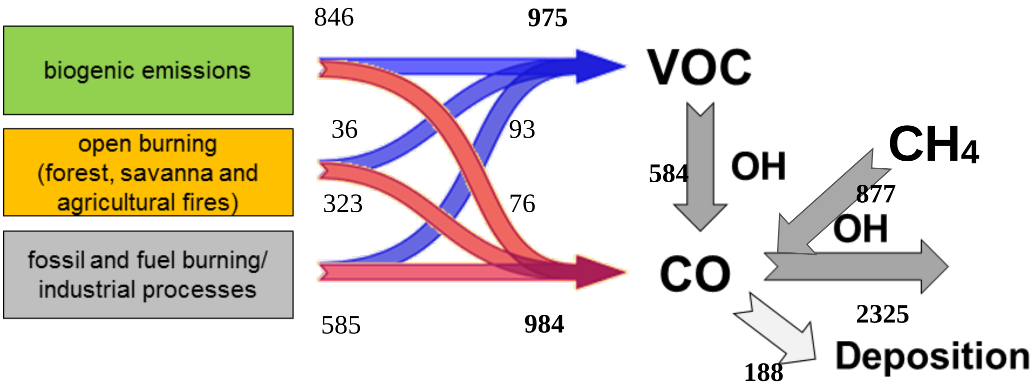

Figure 1: The global CO budget: sources and sinks. Numbers are in Tg y^{-1} as estimated from MOZART-3 using MACCity /MEGAN /GFAS emissions for the year 2008.

In a ECHAM6 climate simulation at MPI-M Hamburg Kracher et al. (2014; 2015) discuss the reduction of the warming potential of N2O by an enhanced Brewer-Dobson circulation (BDC) in a future climate. A particular consequence of the acceleration of the BDC is an enhanced transport of N2O from its sources at the Earth’s surface towards its main sink region in the stratosphere thus inducing a reduction in its lifetime. This leads to a decrease in the N2O global warming potential, which is particularly important in light of climate change mitigation strategies. The simulations reveal a decrease in N2O lifetime by about 7 years K-1 (5.5 % K-1), resulting in a conservative estimate for the reduction of the N2O global warming potential by about 7 CO2-equivalents K-1 (2.4 % K-1). As ECHAM6 does not contain atmospheric chemistry, stratospheric decay rates of N2O are prescribed. Stratospheric decay rates are taken from a MOZART-3 simulation for the year 2008 performed within MACC.

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