SPECIAL PROJECT FINAL REPORT

All the following mandatory information needs to be provided.

Project Title:	Global modelling of atmospheric chemistry
Computer Project Account:	spdeacm
Start Year - End Year :	2015 - 2017
Principal Investigator(s)	Olaf Stein
Affiliation/Address:	Forschungszentrum Jülich JSC / SimLab Climate Science 52425 Jülich Germany
Other Researchers (Name/Affiliation):	Martin Schultz, Florian Berkes, Sabine Griessbach, Sabine Schröder, Snehal Waychal, Yi Heng (all FZJ), Sebastian Rast (MPI-M Hamburg), Angelika Heil (MPI-C Mainz)

The following should cover the entire project duration.

Summary of project objectives

(10 lines max)

- Development of a chemistry module for IFS (CIFS-MOZ)
- Maintenance and development 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 you encountered any problems of a more technical nature, please describe them here.)

none

Experience with the Special Project framework

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

- Transition to new ecmwf websites was not well traceable for outside users
- Some problems with the new ticketing system (communication, login)

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 attachment

List of publications/reports from the project with complete references

List of publications/reports from the project with complete references

Peer-reviewed:

Berkes, F., Neis, P., Schultz, M. G., Bundke, U., Rohs, S., Smit, H. G. J., Wahner, A., Konopka, P., Boulanger, D., Nédélec, P., Thouret, V., and Petzold, A.: In situ temperature measurements in the upper troposphere and lowermost stratosphere from 2 decades of IAGOS long-term routine observation, Atmos. Chem. Phys., 17, 12495-12508, https://doi.org/10.5194/acp-17-12495-2017, 2017.

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., 8, 3523-3543, doi:10.5194/gmd-8-3523-2015, 2015.

Flemming, J., Huijnen, V., Arteta, J., Bechtold, P., Beljaars, A., Blechschmidt, A.-M., Diamantakis, M., Engelen, R. J., Gaudel, A., Inness, A., Jones, L., Josse, B., Katragkou, E., Marecal, V., Peuch, V.-H., Richter, A., Schultz, M. G., Stein, O., and Tsikerdekis, A.: Tropospheric chemistry in the Integrated Forecasting System of ECMWF, Geosci. Model Dev., 8, 975-1003, doi:10.5194/gmd-8-975-2015, 2015.

Gaudel, A., Clark, H., Thouret, V., Jones, L., Inness, A., Flemming, J., Stein, O., Huijnen, V., Eskes, H., Nedelec, P., and Boulanger, D.: On the use of MOZAIC-IAGOS data to assess the ability of the MACC reanalysis to reproduce the distribution of ozone and CO in the UTLS over Europe, Tellus B, 67, 27955, doi:10.3402/tellusb.v67.27955, 2015.

Heng, Y., Hoffmann, L., Griessbach, S., Rößler, T., and Stein, O.: Inverse transport modeling of volcanic sulfur dioxide emissions using large-scale simulations, Geosci. Model Dev., 9, 1627-1645, doi:10.5194/gmd-9-1627-2016, 2016.

Hoffmann, L., T. Rößler, S. Griessbach, Y. Heng, and O. Stein: Lagrangian transport simulations of volcanic sulfur dioxide emissions: Impact of meteorological data products, J. Geophys. Res. Atmos., 121, 4651–4673, doi:10.1002/2015JD023749, 2016

Hoffmann, L., Hertzog, A., Rößler, T., Stein, O., and Wu, X.: Intercomparison of meteorological analyses and trajectories in the Antarctic lower stratosphere with Concordiasi superpressure balloon observations, Atmos. Chem. Phys., 17, 8045-8061, doi.org/10.5194/acp-17-8045-2017, 2017.

Hoffmann, L., Spang, R., Orr, A., Alexander, M. J., Holt, L. A., and Stein, O.: A decadal satellite record of gravity wave activity in the lower stratosphere to study polar stratospheric cloud formation, Atmos. Chem. Phys., 17, 2901-2920, doi:10.5194/acp-17-2901-2017, 2017.

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.

Katragkou, E., Zanis, P., Tsikerdekis, A., Kapsomenakis, J., Melas, D., Eskes, H., Flemming, J., Huijnen, V., Inness, A., Schultz, M. G., Stein, O., and Zerefos, C. S.: Evaluation of near-surface ozone over Europe from the MACC reanalysis, Geosci. Model Dev., 8, 2299-2314, doi:10.5194/gmd-8-2299-2015, 2015.

Kracher, D., C. H. Reick, E. Manzini, M. G. Schultz, and O. Stein, Climate change reduces warming potential of nitrous oxide by an enhanced Brewer-Dobson circulation, Geophys. Res. Lett., 43, doi:10.1002/2016GL068390, 2016.

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.

Liora, N., A. Poupkou, T. M. Giannaros, K. E. Kakosimos, O. Stein, D. Melas: Impacts of natural emission sources on particle pollution levels in Europe, Atmospheric Environment, 137, 171-185, ISSN 1352-2310, http://dx.doi.org/10.1016/j.atmosenv.2016.04.040, 2016.

Lyapina, O., Schultz, M. G., and Hense, A.: Cluster analysis of European surface ozone observations for evaluation of MACC reanalysis data, Atmos. Chem. Phys., 16, 6863-6881, doi:10.5194/acp-16-6863-2016, 2016.

Rößler, T., Stein, O., Heng, Y., Baumeister, P., and Hoffmann, L.: Trajectory errors of different numerical integration schemes diagnosed with the MPTRAC advection module driven by ECMWF operational analyses, Geosci. Model Dev., 11, 575-592, https://doi.org/10.5194/gmd-11-575-2018, 2018.

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.

Stein, O., Schultz, M. G., Bouarar, I., Clark, H., Huijnen, V., Gaudel, A., George, M., and Clerbaux, C.: On the wintertime low bias of Northern Hemisphere carbon monoxide found in global model simulations, Atmos. Chem. Phys., 14, 9295-9316, doi:10.5194/acp-14-9295-2014, 2014.

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., 15, 14005-14030, doi:10.5194/acp-15-14005-2015, 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

Flemming, J., V. Huijnen, J. Arteta, A. Inness, L. Jones, V.-H. Peuch, M. G. Schultz, A.-M. Blechschmidt, A. Richter, O. Stein, R. Engelen, E. Katragou, A. Tsikerdekis, Preliminary documentation of C-IFS code, MACC-II Deliverable D_57.5, July 2014. https://www.gmes-atmosphere.eu/documents/maccii/deliverables/grg/MACCII_GRG_DEL_D57.5_20140725_Flemming.pdf

Hoffmann, L., T. Rößler, S. Griessbach, Y. Heng, O. Stein: Lagrangian transport simulations of volcanic sulfur dioxide emissions: impact of meteorological data products, Geophysical Research Abstracts, Vol. 19, EGU2017-3609, 2017.

Hoffmann, L., A. Hertzog, T. Rößler, O. Stein, X. Wu: Intercomparison of meteorological analyses and trajectories in the Antarctic lower stratosphere with Concordiasi superpressure balloon observations, Geophysical Research Abstracts, Vol. 20, EGU2018-3019, 2018

Hoffmann, L., R. Spang, A. Orr, J. Alexander, L. Holt, O. Stein: A decadal satellite record of gravity wave activity in the lower stratosphere to study polar stratospheric cloud formation, Geophysical Research Abstracts, Vol. 20, EGU2018-3009, 2018

Inness, A., A.-M. Blechschmidt, I. Bouarar, S. Chabrillat, M. Crepulja, R. J. Engelen, H. Eskes, J. Flemming, A. Gaudel, F. Hendrick, V. Huijnen, L. Jones, J. Kapsomenakis, E. Katragkou, A. Keppens, B. Langerock, M. de Mazière, D. Melas, M. Parrington, V.H. Peuch, M. Razinger1, A. Richter, M. G. Schultz, M. Suttie, V. Thouret, M. Vrekoussis, A. Wagner, and C. Zerefos, Data assimilation of satellite retrieved ozone, carbon monoxide and nitrogen dioxide with ECMWF's Composition IFS, Technical Memorandum, 745, Reading, December 2014. http://old.ecmwf.int/publications/library/ecpublications/_pdf/tm/701-800/tm745.pdf

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

Kaiser, J. W., N. Andela, A. Heil, R. Paugam, M. G. Schultz, G. R. van der Werf, M. J. Wooster, Recent developments in Fire Emission Service GFAS in the MACC-II Project, Geophysical Research Abstracts, Vol. 16, EGU2014-16827, 2014.

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.

Kracher, D., C. Reick, E. Manzini, M. Schultz, and O. Stein, Enhanced Brewer Dobson circulation reduces N2O warming potential under climate change, Geophysical Research Abstracts, Vol. 18, EGU2016-14603, 2016.

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

Schultz, M. G., O. Lyapina, S. Schröder, O. Stein, D. Mallmann, and the WMO-ET-WDC, TT-ACV, CAMS, WMO-GAW, TOAR Teams , Linking atmospheric composition data across data types and national boundaries, Geophysical Research Abstracts, Vol. 18, EGU2016-8558, 2016.

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

Stein, O., M. Schultz, M. Rambadt, R. Saini, L. Hoffmann, D. Mallmann: JADDS – towards a tailored global atmospheric composition data service for CAMS forecasts and reanalysis, Geophysical Research Abstracts, Vol. 19, EGU2017-7352, 2017.

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.

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.)

As discussed with DWD and ECMWF, access to ecgate and MARS archive will be further used by accounts so far connected to spdeacm. There will be no application for computer time connected to this activity.

Global modelling of atmospheric chemistry
special project SPDEACM final report (2014-2017)
June 2018

Olaf Stein
Forschungszentrum Jülich

While the years 2014-2015 mostly were devoted to the development of CIFS and the evaluation of the MACC model MOZ-IFS, the years 2016 and 2017 brought major changes to the SPDEACM project: with the shutdown of our modelling activities in CAMS a growing number of publications arose from our scientific work on tracer and meteorological transport modelling, all making extensive use of IFS model output (MACC reanalysis, ERA-Interim, ERA-5). For these purposes, data from historic operational forecasts as well as meteorological and chemical reanalysis products are stored in Jülich for scientific analysis as an ongoing activity. As part of a long-term obligation, data of meteorological and chemical data from the MARS and ECFS archives to the Jülich supercomputing systems is transferred regularly in near-realtime in order to serve our CAMS chemical boundary condition server.

CIFS

In 2014/2015, CIFS-MOZ (Stein and Flemming, 2015) was implemented and updated to IFS cycle 41R1 on ECMWF system cca. SPDEACM participated in two publications describing the CIFS system (Flemming et al., 2015; Inness et al., 2015). After adapting to the new IFS version, we implemented an updated stratospheric chemical scheme. Several longer sensitivity simulations with CIFS in resolution T255 were performed. Beginning of 2016 we decided to shut down our CIFS developments and to abandon the FZJ involvement in CAMS. As a consequence of this decision, no substantial computer allocation was used for the years 2016/2017. The CIFS-MOZ development in CAMS has been handed over to Idir Bouarar (MPI-Met Hamburg).

SPDEACM also contributed to the current pre-operational CAMS 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.

IFS-MOZ

Results from the coupled system IFS-MOZ run in MACC reanalysis and forecasts from 2010 to 2014 have been evaluated and analysed in several scientific papers, which appeared in 2015/16.

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. 1).

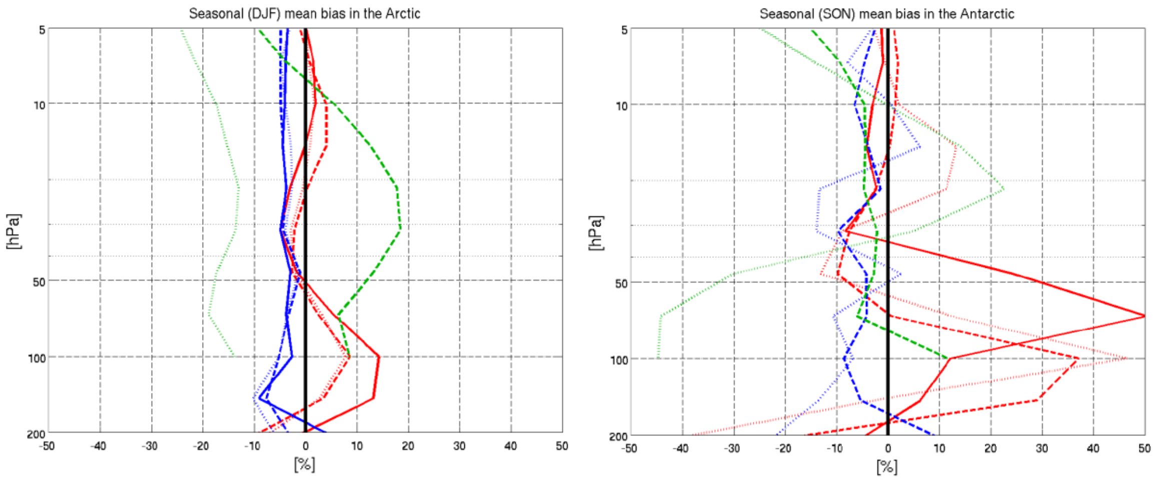

Figure 1: Seasonally averaged relative ozone bias profiles of IFS-MOZART (red), BASCOE (blue), and SACADA (green) versus ACE-FTS (AN minus OBS) in % for the Arctic winter (DJF) 2009-2010 (full), 2010-2011 (dashed), 2011-2012 (dotted) and the Antarctic spring (SON) 2009 (full), 2010 (dashed), and 2011 (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) compare 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 O_3 by 60 ppbv in the lower stratosphere (LS), whilst CO is overestimated by 20 ppbv. In the upper troposphere (UT), O_3 is overestimated by 50 ppbv, but CO is partly over or underestimated by up to 20 ppbv. As expected, assimilation generally improves model results.

Eskes et al. (2015) evaluate reactive gases and aerosols in the MACC global analysis and forecast system simulated with IFS-MOZ during 2012-2014 (MACC o-suite). The paper discusses the approach to validation that has been developed by the MACC VAL group. Topics discussed are the validation requirements, the operational aspects, the measurement data sets used, the structure of the validation reports, the models and assimilation systems validated, the procedure to introduce new upgrades, and the scoring methods. Exemplarily shown here is validation of free tropospheric ozone with respect to combined surface and free tropospheric ozone observations from the GAW network, IAGOS aircraft data, and ozone sondes for different regions (Figure 2).

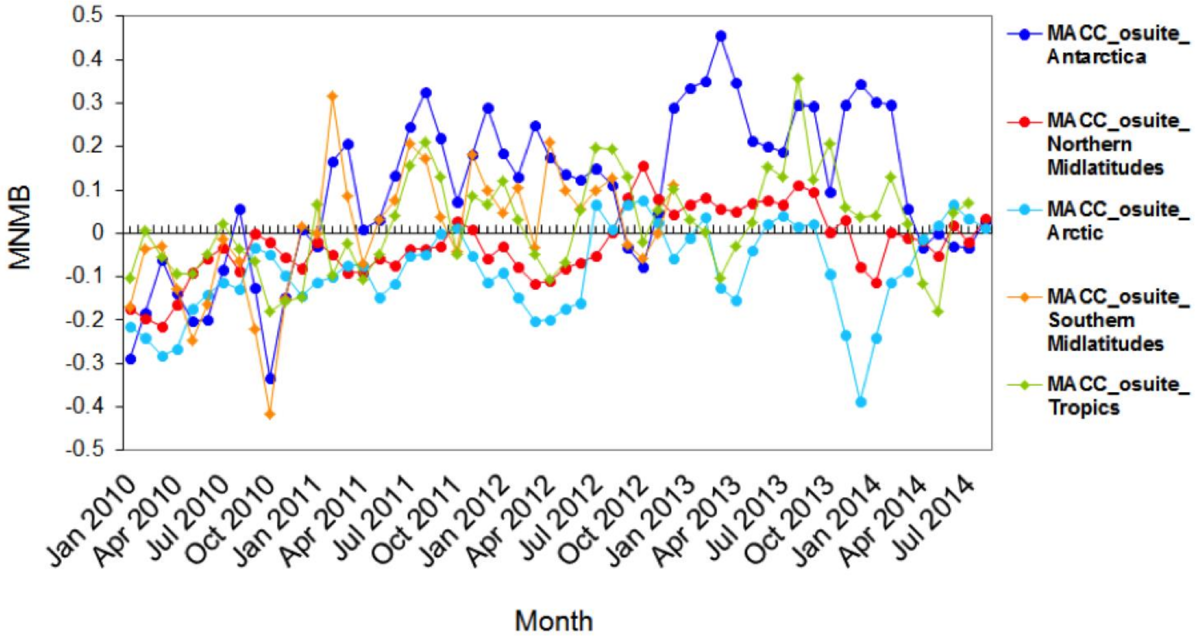

Figure 2: Modified normalized mean bias (MNMB) of ozone in the free troposphere (750–200 hPa) in the tropics and 750–300 hPa elsewhere) of MACC o-suite against aggregated sonde data in four different regions.

Liora et al. (2016) apply chemical boundary conditions from the MACC reanalysis to their regional air quality simulations over Europe with the WRF-CAMx mode.l The main objective of this work is the study of the impact of windblown dust, sea-salt aerosol and biogenic emissions on particle pollution levels in Europe using the novel natural emissions model (NEMO). Air quality simulations were performed for different emission scenarios in order to study the contribution of each natural emission source individually and together to air quality levels in Europe. The exclusion of windblown dust emissions decreases the mean seasonal PM10 levels by more than 3.3 mg/m^3 (~20%) in the Eastern Mediterranean during winter while an impact of 3 mg/m^3 was also found during summer. The results also suggest that sea-salt aerosol has a significant effect on PM levels and composition (Figure 3).

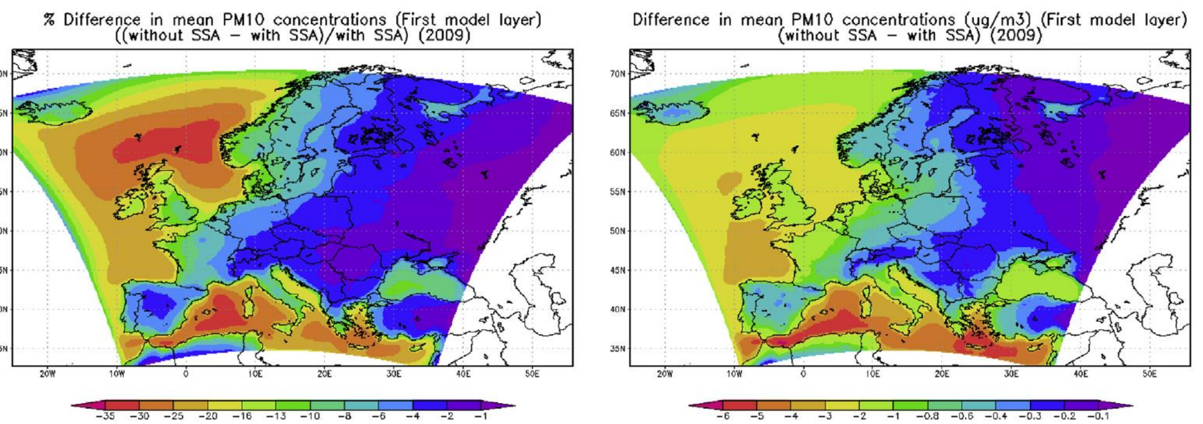

Figure 3: Mean annual percentage contribution (in %) of sea-salt aerosol (SSA) to PM10 levels (left) and mean annual impact of SSA on PM10 levels (in mg/m^3) (right) for 2009.

The MACC reanalysis data is evaluated by means of cluster analysis of European surface ozone observations in a recent paper by Lyapina et al. (2016). In their work, the regional representativeness of European ozone measurements is examined through a cluster analysis of 4 years of 3-hourly ozone data from 1492 European surface monitoring stations in the Airbase database. The individual clusters reveal differences in seasonal–diurnal cycles, showing typical patterns of the ozone behaviour for more polluted stations or more rural background. The seasonal, diurnal, and weekly cycles of each cluster are then compared to the MACC reanalysis. While the MACC reanalysis generally captures the shape of the diurnal cycles and the diurnal amplitudes, it is not able to reproduce the seasonal cycles very well and it exhibits a high bias up to 12 nmol mol^{-1} with a bias decreasing from more polluted clusters to cleaner ones. More generally, it can be shown that relatively coarse-scale global models are more suitable for simulation of regional background concentrations, which are less variable in space and time.

Moreover, a paper on the reduction of the warming potential of nitrous oxide by an enhanced Brewer-Dobson circulation under climate change conditions was published in 2016 (Kracher et al., 2016). Here the implications of a reduced N_2O lifetime in the context of climate change are examined.We find a decrease in the N_2O global warming potential (GWP) and, due to a decline in the atmospheric N_2O burden, also a reduction in its total radiative forcing. From an idealized transient global warming simulation we can identify linear regressions for N_2O sink, lifetime, and GWP with temperature rise. Stratospheric decay rates are taken from a MOZART-3 simulation for the year 2008 performed within the MACC project.

Data services supporting CAMS and MACC

Already since 2012 NRT data from the operational CAMS forecasts (formerly MACC forecasts) as well as from the GFAS fire emission inventory (Kaiser et al. 2012) are transferred to FZ Jülich on a daily basis and made available to the public via our OWS interface JOIN (Waychal et al. 2013; http://join.iek.fz-juelich.de/). In addition, we downloaded all chemical species concentrations from the MACC reanalysis 2003-2012 which are not publically available from the MARS archive. Tracer fields from the CAMS operational forecasts and from the MACC reanalysis are used for scientific analysis of atmospheric chemistry (Gaudel et al., 2015; Lyapina et al, 2016; Kracher et al, 2016) and serve as boundary conditions for regional air quality models (Liora et al., 2016). Currently our existing Web Coverage Service (WCS) for sharing individually tailored model results is being re-engineered to make use of rasdaman, a scalable array database technology in order to improve performance, enhance flexibility, and allow the operation of catalogue services. The WCS protocol is upgraded to WCS2.0 and the metadata shall be interfaced with the EUDAT (https://www.eudat.eu/) service structure (Stein et al., 2017). In 2017, we established a closer collaboration with Julia Wagemann (ECMWF) to share our experiences with access to complex multi-dimensional atmospheric data and with the rasdaman technology also developed at ECMWF in the framework of the EarthServer2 project.

Other studies performed with ECMWF data products

In 2015 we started to use historical operational meteorological data and data from the ERA-INTERIM reanalysis to study the impact of meteorological data products on Lagrangian transport simulations of volcanic sulphur dioxide emissions (Hoffmann et al., 2016). We applied our new Lagrangian transport model Massive-Parallel Trajectory Calculations (MPTRAC) to perform simulations for three case studies of large volcanic eruption events in 2011. Besides validation of the new model, the main goal of the study was a comparison of the simulations with the different meteorological data products ERA-INTERIM, MERRA, and NCEP reanalyses, as well as ECMWF operational analyses. Qualitatively, the SO_2 distributions from the simulations compare well not only with the AIRS data but also with Cloud-Aerosol Lidar with Orthogonal Polarization and Michelson Interferometer for Passive Atmospheric Sounding aerosol observations. During the first 5 or 10 days after the eruptions we found the best performance for the ECMWF analysis by means of the Critical Success Index (CSI) (range of 0.25–0.31), followed by ERA-Interim (0.25–0.29), MERRA (0.23–0.27), and NCAR/NCEP (0.21–0.23).

In a further study by Heng et al. (2016) we performed inverse transport modelling of volcanic sulphur dioxide emissions using large-scale simulations. The approach is based on the concepts of sequential importance resampling and parallel computing in order to reconstruct altitude-resolved time series of volcanic emissions, which often cannot be obtained directly with current measurement techniques. In the inverse modelling system MPTRAC is used to perform two types of simulations, i.e., unit simulations for the reconstruction of volcanic emissions and final forward simulations. Both types of transport simulations are based on wind fields of the ERA-Interim meteorological reanalysis. By using the critical success index (CSI), the simulation results are evaluated with AIRS observations. Compared to the results with an assumption of a constant flux of SO_2 emissions, our inversion approach leads to an improvement of the mean CSI value from 8.1 to 21.4 % and the maximum CSI value from 32.3 to 52.4 %. The simulation results are also compared with those reported in other studies and good agreement is observed.

Small-scale temperature fluctuations induced by atmospheric gravity waves can trigger the formation of polar stratospheric clouds (PSCs). In a study by Hoffmann et al. (2017a) we introduced a new ten-year-long Atmospheric Infrared Sounder (AIRS) satellite record of gravity wave activity in the polar lower stratosphere to investigate this process. The analysis of temporal patterns in the data set revealed a strong seasonal cycle in wave activity with wintertime maxima at mid- and high latitudes. The analysis of spatial patterns indicated that orography as well as jet and storm sources are the main causes of the observed waves. Wave activity is closely correlated with 30 hPa zonal winds, which is attributed to the AIRS observational filter. We used the new data set to evaluate explicitly resolved temperature fluctuations due to gravity waves in the European Centre for Medium-Range Weather Forecasts (ECMWF) operational analysis (Fig. 4). It was found that the analysis reproduces orographic and non-orographic wave patterns in the right places, but that wave amplitudes are typically underestimated by a factor of 2–3.

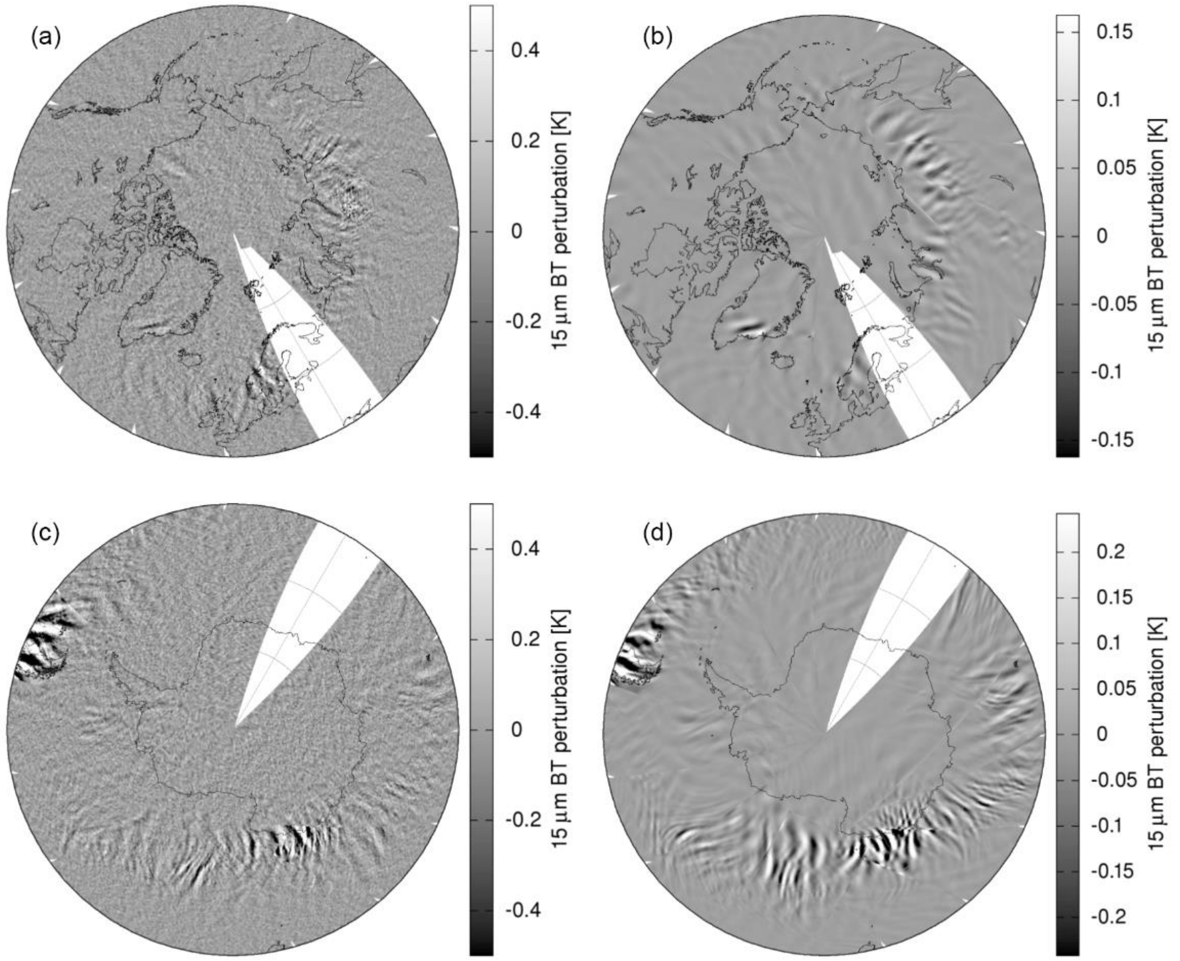

Figure 4: AIRS measurements of 15 µm brightness temperature perturbations (left) and corresponding simulations based on ECMWF operational analysis temperatures (right). Real measurements took place on 11 December 2003 from 12:00 to 24:00 UTC in the Northern Hemisphere (top) and on 22 July 2011 from 00:00 to 12:00 UTC in the Southern Hemisphere (bottom). Simulated measurements are based on synoptic data at 18:00 and 06:00 UTC, respectively.

In a second study by Hoffmann et al. (2017b) we compare temperatures and horizontal winds of meteorological analyses in the Antarctic lower stratosphere. The study covers the ECMWF operational analysis, the ERA-Interim reanalysis, the MERRA and MERRA-2 reanalysis, and the NCEP/NCAR reanalysis. The comparison was performed with respect to long-duration observations from 19 superpressure balloon flights during the Concordiasi field campaign in September 2010 to January 2011 (Fig. 5). Considering the fact that the balloon observations have been assimilated into all analyses, except for NCEP/NCAR, notable differences found in the paper indicate that other observations, different forecast models, and different data assimilation procedures have significant impact on the analyses as well. We also used the balloon observations to evaluate trajectory calculations with our new Lagrangian transport model Massive-Parallel Trajectory Calculations (MPTRAC), where vertical motions of simulated trajectories were nudged to pressure measurements of the balloons.

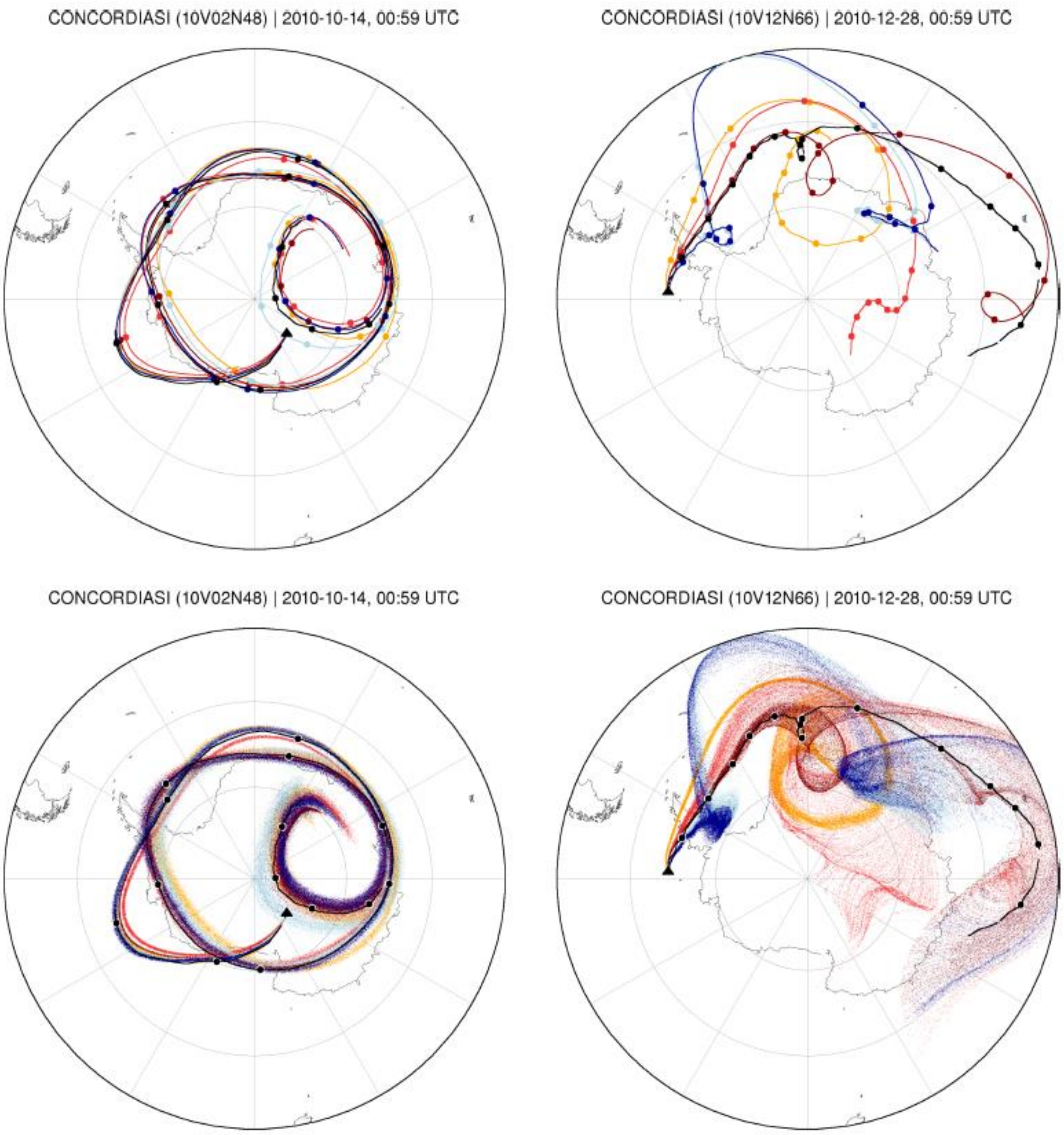

Figure 5: Examples of trajectories calculated with different meteorological analyses (dark blue: ECMWF OA, light blue: ERA-Interim, dark red: MERRA-2, light red: MERRA, orange: NCEP/NCAR) and corresponding Concordiasi balloon trajectory (black). Plot titles provide the starting times and triangles indicate the starting positions of the trajectories. Circles indicate trajectory positions at 0 UTC each day. Plots at the top show individual trajectories calculated without diffusion. Plots at the bottom illustrate dispersion simulations with diffusion being considered.

In a further study by Rößler et al. (2018) we focus on the minimization of truncation errors that originate from the use of numerical integration schemes to solve the kinematic equation of motion. We analysed truncation errors of six explicit integration schemes of the Runge Kutta family, which we implemented in the Massive-Parallel Trajectory Calculations (MPTRAC) model. The simulations were driven by wind fields of ECMWF operational analysis and forecasts at T1279L137 spatial resolution and 3 h temporal sampling. In total more than 5000 different transport simulations were performed and we quantified the accuracy of the trajectories by calculating transport deviations with respect to reference simulations using a 4th-order Runge-Kutta integration scheme with a sufficiently fine time step (Fig. 6). The selection of the integration scheme and the appropriate time step should possibly take into account the typical altitude ranges as well as the total length of the simulations to achieve the most efficient simulations. However, trying to generalize, we recommend the 3rd-order Runge Kutta method with a time step of 170 s or the midpoint scheme with a time step of 100 s for efficient simulations of up to 10 days time based on ECMWF's high-resolution meteorological data.

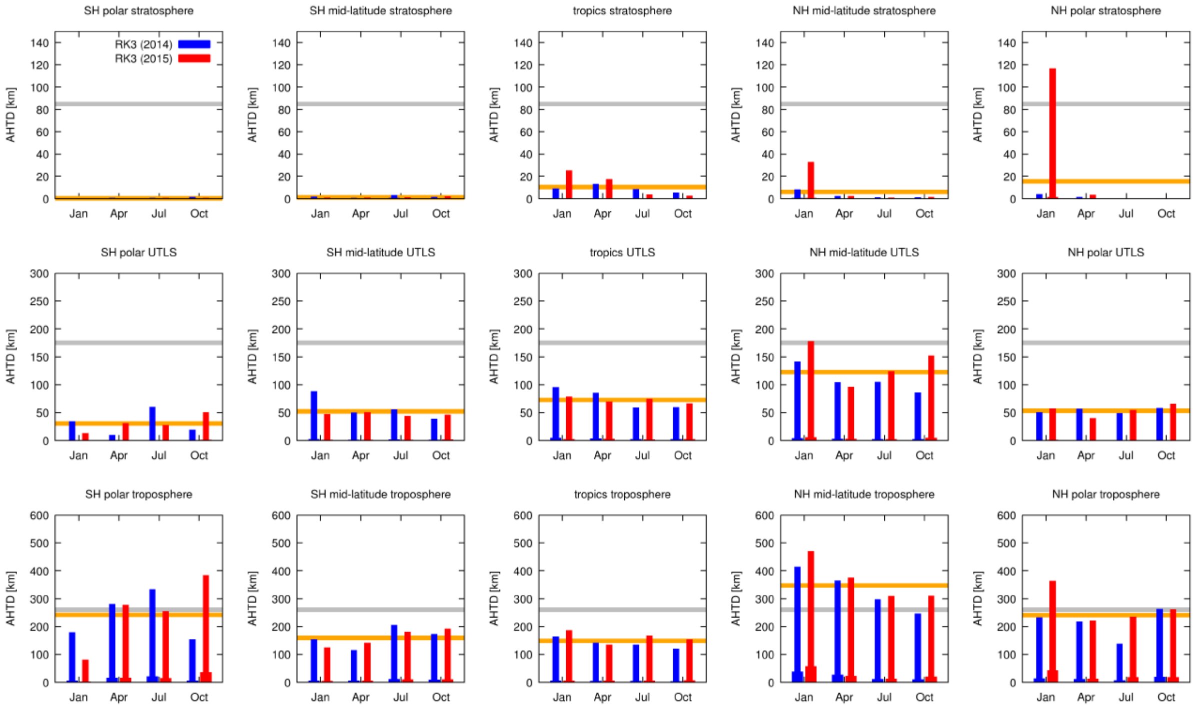

Figure 6: Mean (thin bars) and median (thick bars) horizontal transport deviations after ten days simulation time in different domains for the RK3 method and 120 s time step. Orange lines show the averages of the four months (January, April, July, and October) and both years (2014 and 2015). Gray lines show error limits based on diffusion.

References

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., 8, 3523-3543, doi:10.5194/gmd-8-3523-2015, 2015.

Flemming, J., Huijnen, V., Arteta, J., Bechtold, P., Beljaars, A., Blechschmidt, A.-M., Diamantakis, M., Engelen, R. J., Gaudel, A., Inness, A., Jones, L., Josse, B., Katragkou, E., Marecal, V., Peuch, V.-H., Richter, A., Schultz, M. G., Stein, O., and Tsikerdekis, A.: Tropospheric chemistry in the Integrated Forecasting System of ECMWF, Geosci. Model Dev., 8, 975-1003, doi:10.5194/gmd-8-975-2015, 2015.

Gaudel, A., Clark, H., Thouret, V., Jones, L., Inness, A., Flemming, J., Stein, O., Huijnen, V., Eskes, H., Nedelec, P., and Boulanger, D.: On the use of MOZAIC-IAGOS data to assess the ability of the MACC reanalysis to reproduce the distribution of ozone and CO in the UTLS over Europe, Tellus B, 67, 27955, doi:10.3402/tellusb.v67.27955, 2015.

Heng, Y., Hoffmann, L., Griessbach, S., Rößler, T., and Stein, O.: Inverse transport modeling of volcanic sulfur dioxide emissions using large-scale simulations, Geosci. Model Dev., 9, 1627-1645, doi:10.5194/gmd-9-1627-2016, 2016.

Hoffmann, L., T. Rößler, S. Griessbach, Y. Heng, and O. Stein: Lagrangian transport simulations of volcanic sulfur dioxide emissions: Impact of meteorological data products, J. Geophys. Res. Atmos., 121, 4651–4673, doi:10.1002/2015JD023749, 2016

Hoffmann, L., Spang, R., Orr, A., Alexander, M. J., Holt, L. A., and Stein, O.: A decadal satellite record of gravity wave activity in the lower stratosphere to study polar stratospheric cloud formation, Atmos. Chem. Phys., 17, 2901-2920, doi:10.5194/acp-17-2901-2017, 2017a.

Hoffmann, L., Spang, R., Orr, A., Alexander, M. J., Holt, L. A., and Stein, O.: A decadal satellite record of gravity wave activity in the lower stratosphere to study polar stratospheric cloud formation, Atmos. Chem. Phys., 17, 2901-2920, doi:10.5194/acp-17-2901-2017, 2017a.
Hoffmann, L., Hertzog, A., Rößler, T., Stein, O., and Wu, X.: Validation of meteorological analyses and trajectories in the Antarctic lower stratosphere using Concordiasi superpressure balloon observations, Atmos. Chem. Phys. Discuss., doi:10.5194/acp-2017-71, 2017b.

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.

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.

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 (2011), 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.

Katragkou, E., Zanis, P., Tsikerdekis, A., Kapsomenakis, J., Melas, D., Eskes, H., Flemming, J., Huijnen, V., Inness, A., Schultz, M. G., Stein, O., and Zerefos, C. S.: Evaluation of near-surface ozone over Europe from the MACC reanalysis, Geosci. Model Dev., 8, 2299-2314, doi:10.5194/gmd-8-2299-2015, 2015.

Kracher, D., C. H. Reick, E. Manzini, M. G. Schultz, and O. Stein, Climate change reduces warming potential of nitrous oxide by an enhanced Brewer-Dobson circulation, Geophys. Res. Lett., 43, doi:10.1002/2016GL068390, 2016.

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.

Liora, N., A. Poupkou, T. M. Giannaros, K. E. Kakosimos, O. Stein, D. Melas: Impacts of natural emission sources on particle pollution levels in Europe, Atmospheric Environment, 137, 171-185, ISSN 1352-2310, http://dx.doi.org/10.1016/j.atmosenv.2016.04.040, 2016.

Lyapina, O., Schultz, M. G., and Hense, A.: Cluster analysis of European surface ozone observations for evaluation of MACC reanalysis data, Atmos. Chem. Phys., 16, 6863-6881, doi:10.5194/acp-16-6863-2016, 2016.

Rößler, T., Stein, O., Heng, Y., Baumeister, P., and Hoffmann, L.: Trajectory errors of different numerical integration schemes diagnosed with the MPTRAC advection module driven by ECMWF operational analyses, Geosci. Model Dev., 11, 575-592, https://doi.org/10.5194/gmd-11-575-2018, 2018.

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.

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

Stein, O., M. Schultz, M. Rambadt, R. Saini, L. Hoffmann, D. Mallmann: JADDS – towards a tailored global atmospheric composition data service for CAMS forecasts and reanalysis, Geophysical Research Abstracts,
Vol. 19, EGU2017-7352, 2017.

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.

Waychal, S., M. Schultz, M. Decker, S. Lührs, S. Schröder, O. Stein, JOIN: Jülich OWS Interface, Geophysical Research Abstracts, Vol. 15, EGU2013-8949, 2013.