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 2014/2015

Project Title: Monitoring Atmospheric Composition and Climate - Phase 3 (MACC-III)

Computer Project Account: SP DEFRIU

Principal Investigator(s): Hendrik Elbern

Affiliation: Rhenish Institute for Environmental Research at the University of Cologne (RIUUK)

Name of ECMWF scientist(s) collaborating to the project (if applicable) Vincent-Henri Peuch

Start date of the project: July 2014

Expected end date: June 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)	2,250,000	2,248,000	2,420,000	1,100,000
Data storage capacity	(Gbytes)	14,600	4,500	3,300	1,700

Summary of project objectives

The overall objective of MACC-III (Monitoring Atmospheric Composition and Climate – Phase 3) is to function as the bridge between the project MACC-II and the Atmosphere Service envisaged to form part of Copernicus Operations and expected to start in autumn 2015. MACC-III sustains the current pre-operational atmosphere activities until end of June 2015 in order to avoid any interruption in the critical handover phase between the pre-operational and fully operational service. Thus, at least in 2016 and 2017 this special project will be devoted to the fully operational Copernicus Atmosphere Monitoring Service (CAMS).

Summary of problems encountered

End of 2014 we run out of computing time due to the use of a computational demanding module for the computation of biogenic emissions for the prototype operational air quality forecast.

Summary of results of the current year (from July of previous year to June of current year)

The scientific plan of this special project is fully based on the corresponding concept of MACC-III, as it is detailed in the Description of Work in more comprehensive terms.
The Rhenish Institute for Environmental Research at the University of Cologne (RIUUK) is leading subproject EDA (*Data assimilation for European air quality*) and takes an active part in sub-projects ENS (*Ensemble air quality forecasts for Europe*), EVA (*Validated Assessments of air quality for Europe*), and GRG (*Global reactive gases*) of MACC-III.
All simulations described in this report were done with the EURopean Air pollution Dispersion – Inverse Model (EURAD-IM, Elbern et al., 2007).

1 Data Assimilation for European Air Quality (EDA)

EDA aims to ensure an optimal exploitation of information contents from all available in situ or space born observations. In MACC-III EDA seeks to extend the suite of data from sensors, which were not considered so far for assimilation by RIUUK.

1.1 IASI O_3 and CO data assimilation

IASI is an infrared Fourier transform spectrometer developed jointly by CNES (the French spatial agency), and by EUMETSAT. IASI is mounted on-board the European polar-orbiting MetOp satellite. It contributes to atmospheric composition measurements for climate and chemistry applications with high horizontal resolution and sampling, and with 1 km vertical resolution (Clerbaux et al., 2009). To reach this objective, IASI measures the infrared radiation of the Earths surface and of the atmosphere between 645 and 2760 cm^{-1} at nadir and along a 2200 km swath perpendicular to the satellite track. A total of 120 views are collected over the swath, divided as 30 arrays of 4 individual Field-of-views varying in size from $36 \times \pi$ km^2 at nadir (circular 12 km diameter pixel) to $10 \times 20 \times \pi$ km^2 at the larger viewing angle. IASI offers in this standard observing mode global coverage twice daily, with overpass times at around 9:30 and 21:30 mean local solar time.

An observation operator and its adjoint for FORLI (Fast Optimal Retrievals on Layers for IASI) (Hurtmans et al., 2012) O_3 columns have been developed and integrated in the EURAD-IM assimilation system. FORLI provides partial O_3 columns for 19 atmospheric layers. Levels 1 to 18 correspond to 18 atmospheric layers with 1 km thickness, level 19 to the layer from 18 to 60 km. The observation operator computes model equivalents of O_3 partial columns for these layers between the surface and the model top at 100 hPa.

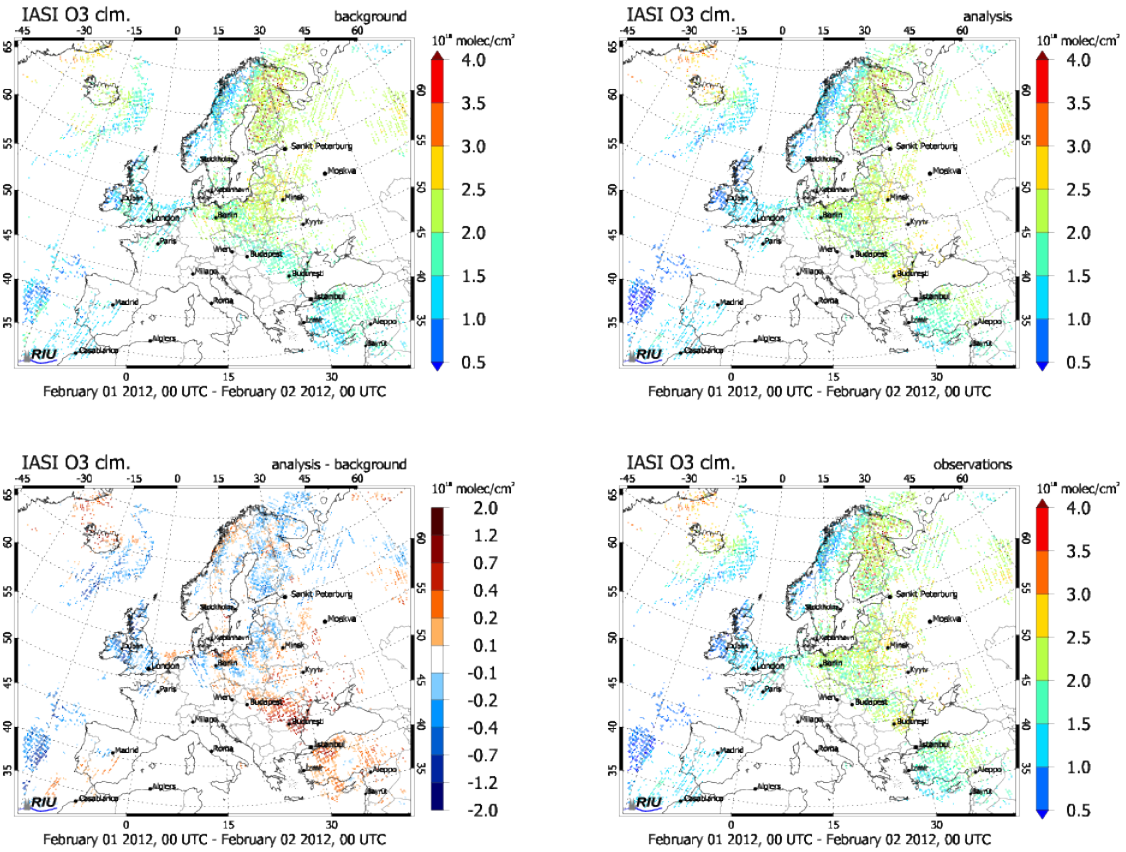


Figure 1: FORLI partial O3 columns integrated between the surface and 100 hPa for February 1, 2012. Upper left: EURAD-IM forecast without data assimilation, upper right: EURAD-IM analysis, lower left: differences between analysis and forecast, lower right: observations.

The 3d-var assimilation of FORLI O_3 data were tested for two episode types, an episode with high Ozone concentrations from July 7 - 16, 2010 and a case with high particulate matter concentrations from January 16 to February 3, 2012. Figure 1 shows FORLI partial O_3 columns for 1. February 2012. The assimilation of IASI O_3 data was independently validated with Ozonesonde measurements. Figure 2 shows Ozone profiles at Uccle for 27. January 2012. The assimilation of FORLI O_3 data has clearly improved the skill of EURAD-IM to simulate upper tropospheric Ozone concentrations. The improvement of near-surface concentrations originates from the assimilation of surface in situ measurements.

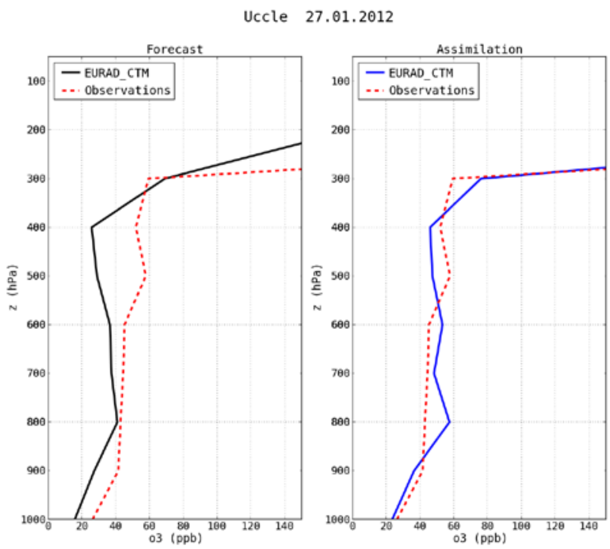


Figure 2: Ozone profiles at Uccle for January 27, 2012. Black: EURAD-IM forecast, blue: EURAD-IM analysis, red: observations.

An observation operator for FORLI CO data and its adjoint has been developed and was integrated in the EURAD-IM assimilation system. In a first step, the observation operator computes CO partial columns for all FORLI layers between the surface and the model top at 100 hPa. Finally, the FORLI averaging kernel vector for the partial columns is applied to compute the model equivalent. Figure 3 shows results from a 3d-var assimilation experiment of IASI FORLI-CO data for March 25, 2013. The EURAD-IM background CO columns do not have a general bias: at March 25 the CO column content was rather over estimated in north-east Europe and under estimated in south-east Europe. The bias was significantly reduced in the analysis run.

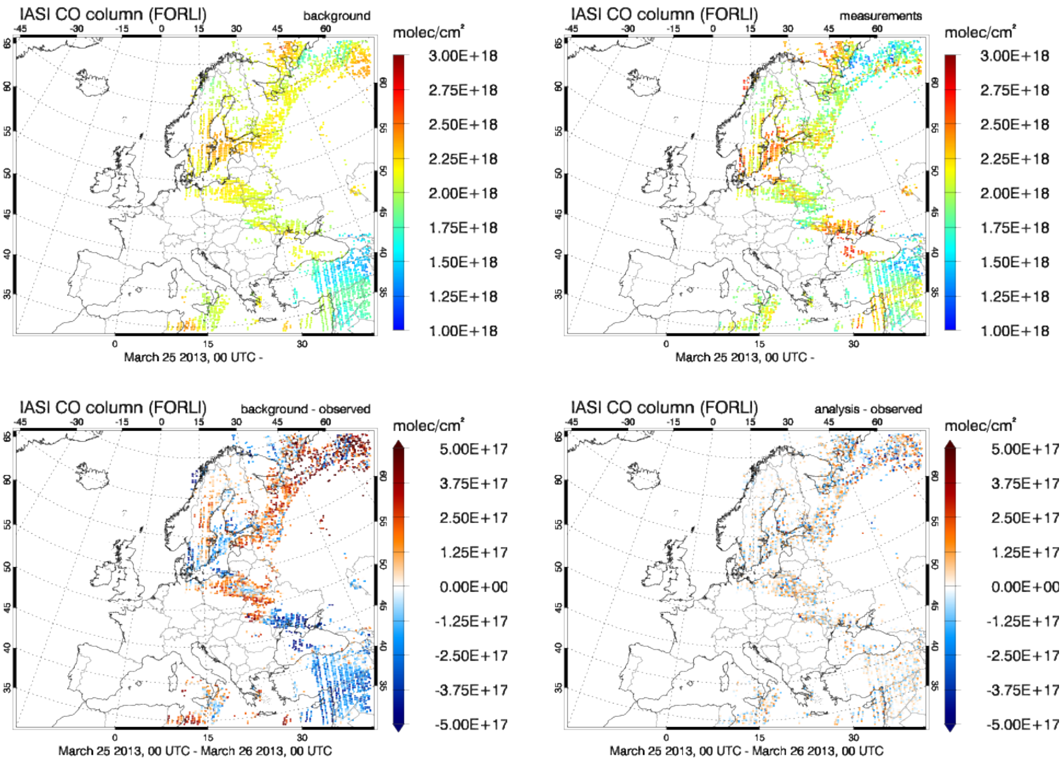


Figure 3: Atmospheric CO columns (below 100 hPa) for March 25, 2013. Upper left: background model equivalents, upper right: IASI FORLI-CO data, lower left: background minus measurements, lower right: analysis minus measurements.

1.2 3d-var assimilation of MODIS AOD measurements

The EURAD-IM assimilation system has been extended by observation forward and adjoint operators for the aerosol optical depth at 550 nm. Aerosol particles are treated as internally mixed. Refractive indices of the individual aerosol species (Schroedter-Homscheidt, 2010) are averaged according to their weight fraction. Inorganic aqueous species are merged to one component whose refractive index is computed with the Biermann (2000) mixing rule. A fast approximation according to Evans and Fournier (1990) in combination with a 50 point Gauss-Legendre quadrature is used for the calculation and integration of the extinction efficiency with respect to particle size.

The observation operator was applied on MODIS AOD measurements in a 3d-var assimilation experiment. Figure 4 shows model equivalents of the aerosol optical depth at 550 nm for March 24, 2013. The assimilation has strongly improved high AOD values measured over the Mediterranean Sea south of Italy, which most probably originate from a Sahara dust outbreak. In some areas e.g. over the Baltic Sea AOD values are over estimated in the analysis. We suppose that this over estimation is an implication of the truncation of the aerosol water gradient. The consideration of aerosol water is necessary for the construction of an accurate adjoint AOD observation operator. However, in the assimilation procedure the aerosol water gradient is set to zero because aerosol water is currently not a prognostic variable of the EURAD-IM aerosol module.

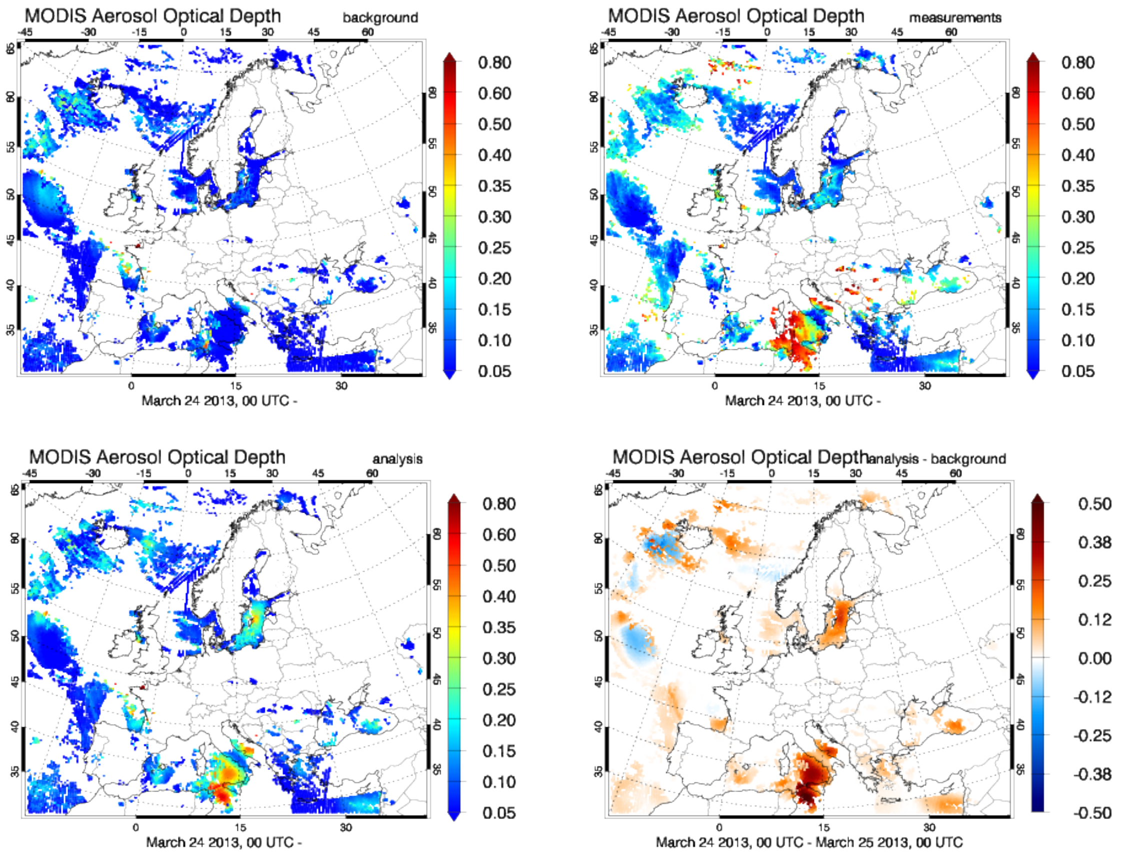


Figure 4: AOD at 550 nm for March 24, 2013. Upper left: background model equivalent, upper right: MODIS measurements, lower left: analysis model equivalent, lower right: analysis minus background.

1.3 Volcanic emission data assimilation

The EURAD-IM is applying a derivative of its mineral dust module with a volcanic eruption column simulator, to account for a flexible height and time source function. In addition to AOD retrieval systems integrated in EURAD-IM earlier, a lidar observation operator for ground based and satellite borne (CALIOP) data has been installed. The system has been applied and validated for the Eyjafjöll 2010 and Etna December 2013 eruption, the latter being a voluntary contribution to the ESA VAST project.

From end of August 2014 until March 2015 a fissure in the Holuhraun lava field on Iceland was continuously erupting rather effusively with a large and continuous flow of lava and a significant release of sulphur dioxide (SO_2) into the lower troposphere. For the whole period, daily forecasts of volcanic SO_2 dispersion are produced for the European region (15 km horizontal grid resolution) and the results are published on our website (http://apps.fz-juelich.de/iek-8/RIU/Index_en.php).

In September 2014 several European measurement sides recorded extremely high SO_2 concentrations at ground level which were predicted quite accurately in advance by the EURAD-IM (see Figure 4). Furthermore, the simulations indicate that the unusual high SO_2 values are due to the transport of SO_2 rich air from Holuhraun towards continental Europe.

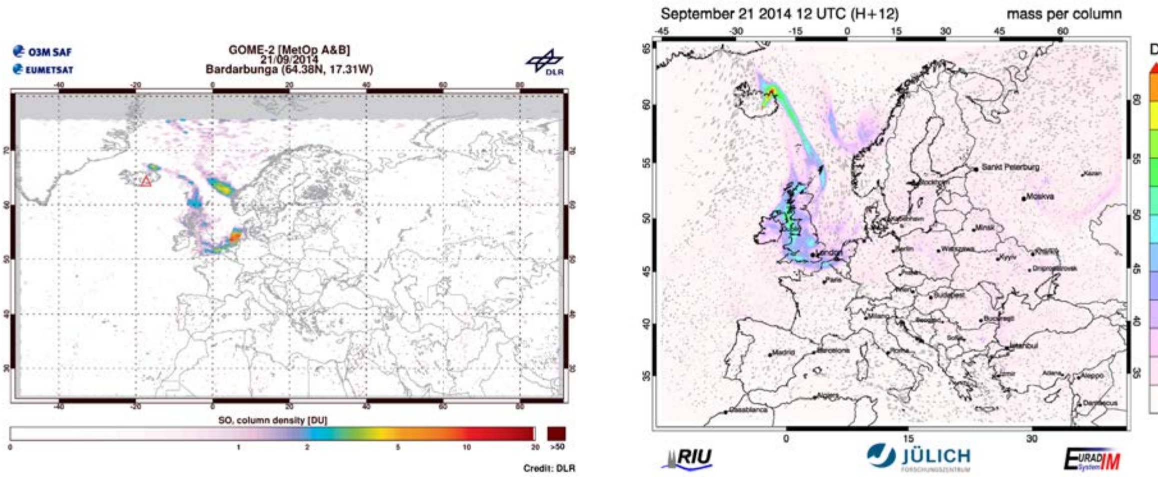


Figure 5: SO_2 vertical column density, 21.09.2014. Left: GOME-2 measurements (source: DLR), right: EURAD-IM forecast at 12:00 UTC.

2. Ensemble Air-Quality Forecasts for Europe (ENS)

ENS primarily focuses on the delivery and verification of the operational European-scale regional NRT air-quality services. In direct continuation from MACC and MACC-II, this service is based upon an ensemble of forecasts performed at seven centres in Europe, including RIUUK. Anymore ENS includes a component that aims to continuous further development of the forecast model.

2.1 Air-quality forecasts

This task corresponds to the prototype operational provision of forecasts for key air-quality compounds with the EURAD-IM system up to 96h for a range of molecules and vertical levels in GRIB2 format. Core products of MACC-II were forecasts of O_3, NO, NO_2, SO_2, CO, $PM_{2.5}$, and PM_{10} at the surface level and at 500, 1000, and 3000 m height. These core products are verified at the surface on a daily NRT basis. Following a request of MACC users, the forecast products have been amended by concentrations of NH_3, NMVOC, and total PAN. The vertical resolution of the forecast products has been increased by additional provision of data at 50, 250, 2000, and 5000 m height. Each year starting at the beginning of March Birch pollen forecasts are provided.

2.2 Air-quality analyses

This task corresponds to the prototype operational provision of analyses for key air-quality compounds (O_3, NO, NO_2, SO_2, CO, $PM_{2.5}$, and PM_{10}) with EURAD-IM. Hourly analyses for the previous day are delivered daily. At first, this is done every day in the early morning with a reduced set of surface in situ observations to provide improved initial values for the subsequent forecast. A second analysis of the previous day has been set up at 08:00 UTC, which includes as many as possible NRT observations. Currently these are surface in situ observations from the EEA, OMI and GOME-2 NO_2 columns, and MOPITT CO profile retrievals.

2.3 Development of the EURAD-IM model

A new development on regional carbon dioxide modelling has been undertaken, in view of potential future high-resolution surface CO_2 flux inversion products over Europe. Due to the high variability in space and time of CO_2 fluxes, it is *a priori* interesting to investigate potential new regional services, complementing the ones provided for the global scale.

Anthropogenic emissions are derived from the TNO inventory for the reference year 2005, supplying point and area sources of CO_2 for Europe divided in 10 source categories. Figure 6 shows traffic related emissions for central Europe.

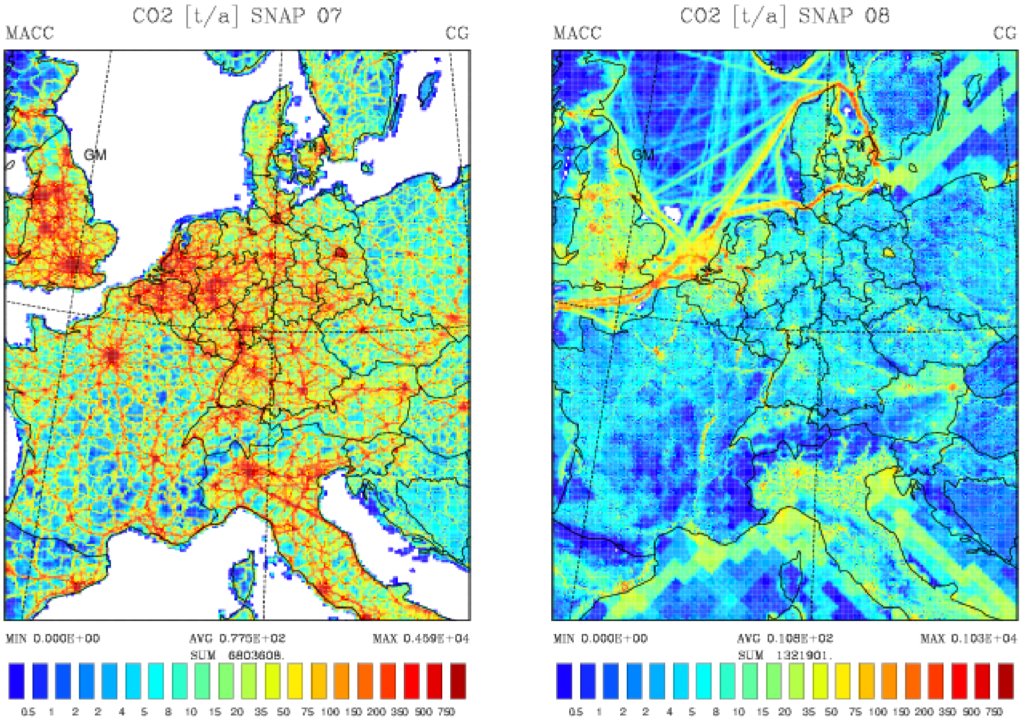


Figure 6: TNO CO_2 emissions for road transport (left) and other mobile sources (right).

The biogenic fluxes are calculated with the Weather Research and Forecasting (WRF) Model (Version 3.6.1) using the Community Land Model (CLM4.0) as land surface model. While photosynthesis is already included in this configuration, leaf respiration has been implemented according to Collatz et al. (1991) and soil respiration has been implemented as an Arrhenius type equation (Lloyd and Taylor, 1994). The calculation of photosynthesis and leaf respiration uses the averaged monthly MODIS leaf area index given by WRF (see Figure 7). To improve the modeling of the passive tracer CO_2 an absolute monotone advection scheme (Walcek, 2000) has been implemented in the EURAD-IM CTM. This prevents spurious wiggles occurring at sharp spatial gradients of CO_2 concentrations (e.g. close to strong anthropogenic point sources). Due to the low numerical diffusion of the Walcek scheme, many structures of anthropogenic sources and biogenic fluxes are resolved in the lowest layer of the atmospheric CO_2 concentration (see Figure 8).

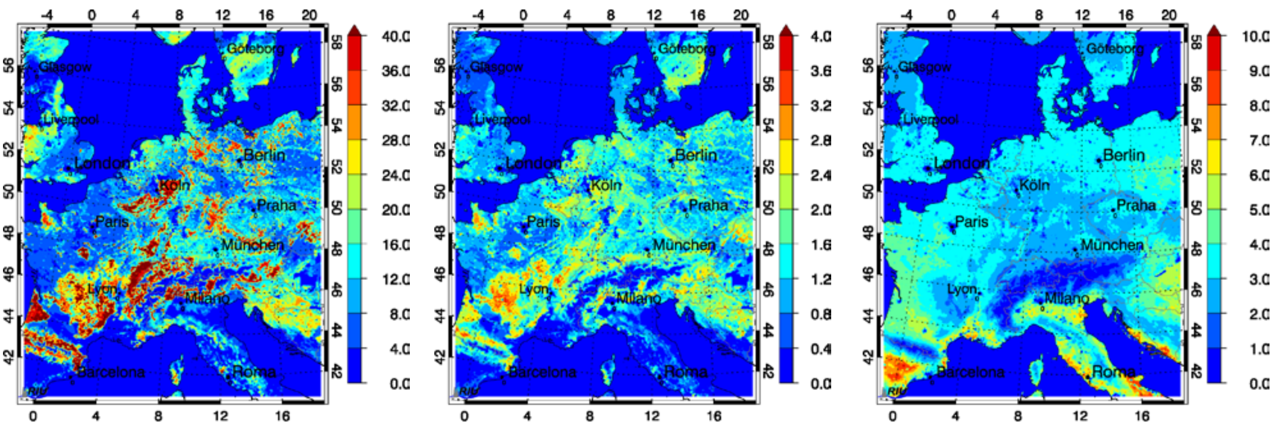


Figure 7: biogenic CO_2 flux for July 23, 2012 13:00 UTC, from left to right: photosynthesis, leaf respiration, soil respiration.

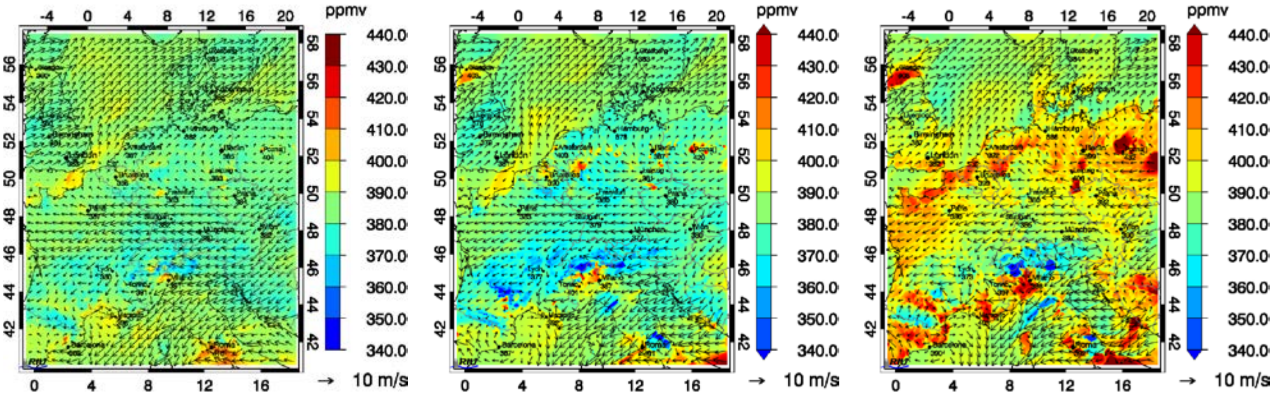


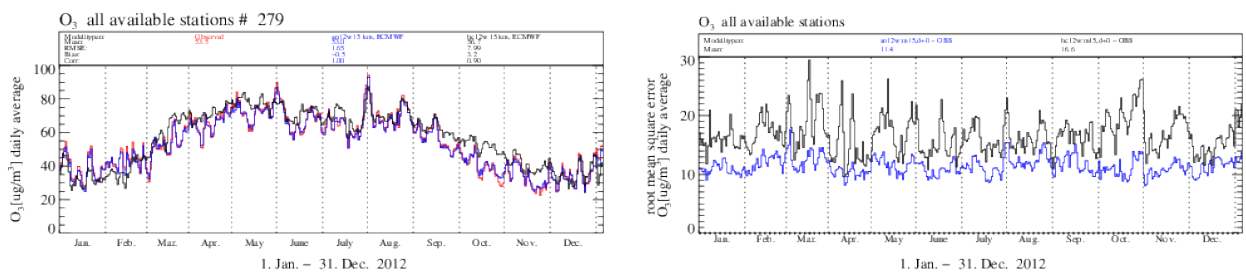
Figure 8: near-surface CO_2 concentration for July 23, 2015 at 12:00 UTC (left), 18:00 UTC (middle), and 22:00 UTC (right).

3. Validated Assessments of Air Quality for Europe (EVA)

Objectives of the EVA sub-project are the development and the implementation of an operational process dedicated to the yearly production of air quality assessment reports that describe air quality in Europe. The state and the evolution of background concentrations of air pollutants in Europe are described in these reports. Validated observation and modeling data are combined in re-analysed numerical fields and maps, to propose the best available representation of air pollutant concentration fields for a spatial resolution of 0.1 deg.

Validated assessment reports from EVA are based upon an ensemble of models hosted at seven institutions in Europe, including RIUUK. During the accounting period the 2012 air quality re-analysis was completed. In situ data from the AIRBASE measurement database maintained by the European Environment Agency (EEA), and NO_2 column retrievals from OMI and GOME-2 were assimilated every hour using the intermittent 3d-var technique. About 30% of surface in situ background stations were used for an independent validation of the assimilation. Figure 9 shows bias and root mean square error of daily averaged O_3, NO_2, SO_2, PM_{10}, and $PM_{2.5}$ concentrations averaged over all Airbase background measurement sites, which were held back from assimilation for the year 2012. The period from end of January to mid of February 2012 was characterized by unusual high SO_2 and PM concentrations over wide areas of Middle Europe. The EURAD-IM forecast was not able to reproduce these high concentrations. In the re-analysis the large negative bias has been significantly reduced.

Some constrains related to the availability of validated regulatory observation data from the EAA, appeared to be an issue for the publication of the EVA reports within a period shorter than two years. MACC-III has given the opportunity to assess the feasibility of the publication of "interim reports" in a shorter time. An assessment of the European air quality for the year 2013 based on "non-fully validated" observation data (in the sense of the air quality directive reporting process) was provided. The EURAD-IM re-analysis was again member of the ensemble used for this assessment.



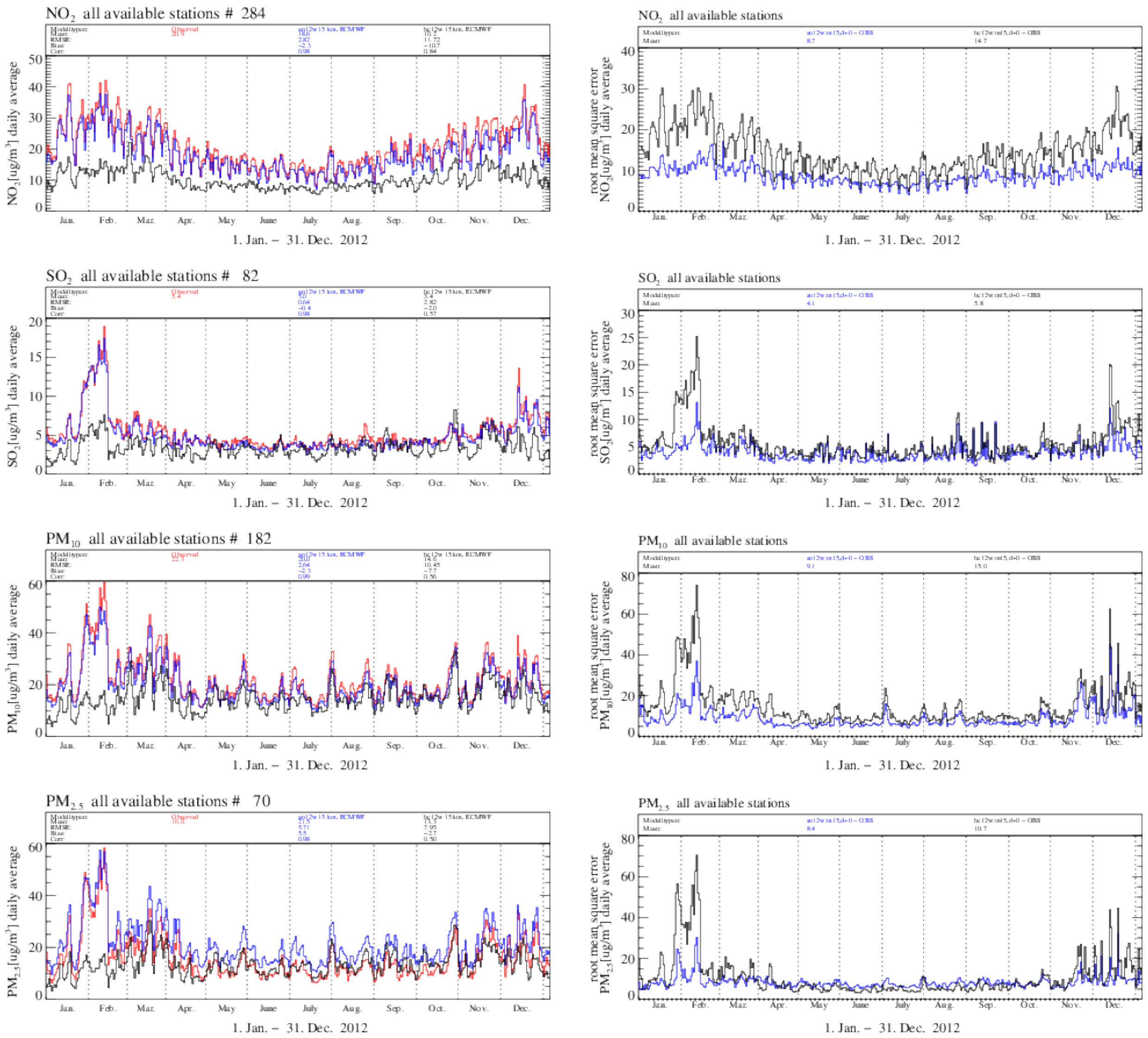


Figure 9: Daily averaged concentration (left) and its root mean square error (right) of O_3 (first row), NO_2, SO_2, PM_{10}, and $PM_{2.5}$ (last row) averaged over all AIRBASE measurement sites, which were held back from assimilation for the year 2012. Red: observations, blue: EURAD-IM 3d-var re-analysis, 30% of stations held back from assimilation, black: control run (no data assimilation at all).

References

Biermann, U.M., B.P. Luo, and T. Peter, Absorption spectra and optical constants of binary and ternary solutions of H_2SO_4, HNO_3, and H_2O in the mid infrared at atmospheric temperatures, *J. Phys. Chem. A*, **104**, 783-793, 2000.

Clerbaux, C., A. Boynard, L. Clarisse, M. George, J. Hadji-Lazaro, H. Herbin, D. Hurtmans, M. Pommier, A. Razavi, S. Turquety, C. Wespes, P.-F. Coheur: Monitoring of atmospheric composition using the thermal infrared IASI/MetOp sounder, *Atmos. Chem. Phys.*, **9,** 6041-6054, 2009, doi: 10.5194/acp-9-6041-2009.

Collatz, G J., J.T. Ball, C. Grivet, J.A. Berry, Physiological and environmental regulation of stomatal conductance, photosynthesis and transpiration: A model that includes a laminar boundary layer, *Agricultural and Forest Meteorology*, **54** (2), 107-136, 1991.

Elbern, H., A. Strunk, H. Schmidt, and O. Talagrand, Emission rate and chemical state estimation by 4-dimensional variational inversion, *Atmos. Chem. Phys*., **7** (2007), 1-59, 2007.

Evans, T.N. and G.R. Fournier, Simple approximation to extinction efficiency valid over all size parameters, *Applied Optics*, 29, 4666-4670, 1990.

Hurtmans, D., P.-F. Coheur, C. Wespes, L. Clarisse, O. Scharf, C. Clerbaux,, A., J. Hadji-Lazaro, M. George, S. Turquety, FORLI radiative transfer and retrieval code for IASI, *J. Quant. Spectrosc. Radiat. Transf.*, **113**, 1391-1408, 2012.

Lloyd, J. and J.A. Taylor, On the temperature dependence of soil respiration. In: Functional ecology, S. 315-323, 1994.

Schroedter-Homscheidt, M., H. Elbern, and T. Holzer-Popp, Observation operator for the assimilation of aerosol type resolving satellite measurements into a chemical transport model, *Atmos. Chem. Phys.*, **10**, 10435-10452, doi:10.5194/acp-10-10435- 2010, 2010.

Walcek, C.: Minor flux adjustment near mixing ratio extremes for simplified yet highly accurate monotonic calculation of tracer advection, *J. Geophys. Res.*, **105 (D7)**, 9335-9348, 2000.

List of publications/reports from the project with complete references

Marécal., V., V.-H. Peuch, C. Andersson , S. Andersson, J. Arteta, M. Beekmann, A. Benedictow, R. Bergström, B. Bessagnet, A., Cansado, F. Chéroux, A. Colette, A. Coman, R.L. Curier, H. A. C. Denier van der Gon, A Drouin, H. Elbern, E. Emili, R. J. Engelen, H. J. Eskes, G. Foret, E. Friese, M. Gauss, C. Giannaros, M. Joly, E. Jaumouillé, B. Josse, N. Kadygrov, J. W. Kaiser, K. Krajsek, J. Kuenen, U. Kumar, N. Liora, E. Lopez, L. Malherbe, I. Martinez, D. Melas, F. Meleux, L. Menut, P. Moinat, T. Morales, J. Parmentier, A. Piacentini, M. Plu, A. Poupkou, S. Queguiner, L. Robertson, L. Rouïl, M. Schaap, A. Segers, M. Sofiev, M. Thomas , R. Timmermans, Á. Valdebenito, P. van Velthoven, R. van Versendaal, J. Vira, A. Ung, A regional air quality forecasting system over Europe : the MACC-II daily ensemble production, *Geosci. Mod. Dev. Discuss*, **8**, 2739-2806, 2015.

Sofiev. M., U. Berger, M. Prank, J. Vira, J. Arteta, J. Belmonte, K.-C. Bergmann, F. Cheroux, H. Elbern, E. Friese, C. Galan, R. Gehrig, R. Kranenburg, V. Marécal, F. Meleux, A.-M. Pessi, L. Robertson, O. Ritenberga, V. Rodinkova, A. Saarto, A. Segers, E. Severova, I. Sauliene, B. M. Steensen, E. Teinemaa, M. Thibaudon, V.-H. Peuch, Multi-model simulations of birch pollen in Europe by MACC regional ensemble, *Atmos. Chem. Phys. Discuss*., **15**, 8243-8281, 2015.

Bocquet, M., Elbern, H., Eskes, H., Hirtl, M., Žabkar, R., Carmichael, G. R., Flemming, J., Inness, A., Pagowski, M., Pérez Camaño, J. L., Saide, P. E., San Jose, R., Sofiev, M., Vira, J., Baklanov, A., Carnevale, C., Grell, G., and Seigneur, C.: Data assimilation in atmospheric chemistry models: current status and future prospects for coupled chemistry meteorology models, Atmos. Chem. Phys. Discuss., 14, 32233-32323, doi:10.5194/acpd-14-32233-2014, 2014.

Hoppe, C. M., Elbern, H., and Schwinger, J.: A variational data assimilation system for soil–atmosphere flux estimates for the Community Land Model (CLM3.5), Geosci. Model Dev., 7, 1025-1036, doi:10.5194/gmd-7-1025-2014, 2014.

Li, Y.P., H. Elbern, K. D. Lu, E. Friese, A. Kiendler-Scharr, Th. F. Mentel, X. S. Wang, A. Wahner, and Y. H. Zhang, Updated aerosol module and its application to simulate secondary organic aerosols during IMPACT campaign May 2008, accepted for publication in ACP, Atmos. Chem. Phys. Discuss., 13, 5961-6005, 2013, doi:10.5194/acpd-13-5961-2013.

Goris, N., and H. Elbern
Singular vector decomposition for sensitivity analyses of tropospheric chemical scenarios
Atmos. Chem. Phys., 13, 5063-5087, 2013.

Summary of plans for the continuation of the project

In November 2014, the European Commission signed a Delegation Agreement with ECMWF for the implementation of CAMS. A procurement process has been recently initiated. At the current state only limited information about the topic of the individual sub-projects is available. The service will be fully operational in the second half of 2015. The Rhenish Institute for Environmental Research intends to contribute to sub-projects CAMS 50 (Regional Production), CAMS 61 (Development of regional air quality modeling aspects), and CAMS 62 (Development of regional air quality data assimilation aspects).