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	2015/2016
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

Please answer for all project resources

		Previous year		Current year	
		Allocated	Used	Allocated	Used
High Performance Computing Facility	(units)	2,420,000	2,143,000	2,600,000	980,000
Data storage capacity	(Gbytes)	3,300	3,400	3,300	1,700

Summary of project objectives

In October 2015 the project MACC-III (Monitoring Atmospheric Composition and Climate – Phase 3) went over to the fully operational Copernicus Atmosphere Monitoring Service (CAMS). CAMS provides continuous data and information on atmospheric composition. The service describes the current situation, forecasts the situation a few days ahead, and analyses consistently retrospective data records for recent years. CAMS has been developed to support policymakers, business and citizens with enhanced atmospheric environmental information. The Rhenish Institute for Environmental Research at the University of Cologne (RIUUK) plays an active role in subproject CAMS 50.

This special project is mainly dedicated to scientific aspects of CAMS 50 based on the corresponding concept of MACC-III, as it is detailed in the Description of Work in more comprehensive terms.

Summary of problems encountered

No problems encountered during the reporting period.

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

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

1.1 Joint flux and state CO_2 optimization with the 4D-Var model EURAD-IM

Regional atmospheric CO_2 inversions seek to reduce uncertainties of CO_2 surface fluxes - anthropogenic CO_2 emissions, photosynthesis, and respiration - with the additional information of atmospheric concentration measurements and the usage of adjoint transport models. With increasing spatial-temporal resolution the uncertainty of atmospheric inversions is also increasing due to two reasons (Lauvaux et al., 2008). First the spatial heterogeneity of European land use impedes proper carbon surface fluxes (Peters et al., 2010). Second, uncertainty of atmospheric transport may lead to several ppm CO_2 due to advection (Lin and Gerbig, 2005) and vertical mixing (Gerbig et al., 2008), which is considerably higher during night (Dolmann et al., 2009; Kretschmer et al., 2014).

We try to improve the analysis and forecast of surface carbon fluxes as we take uncertainty of CO_2 mixing ratios during sunrise also into account and optimize initial values and carbon fluxes jointly. Anthropogenic emissions are taken from the TNO MACC-III inventory for the year 2011. Hourly biogenic fluxes are calculated with the Community Land Model (CLM, version 4.0, Oleson et al., 2010), used as land surface scheme for WRF (Version 3.6.1). While photosynthesis is already included in this configuration, leaf respiration is implemented according to Collatz et al. (1991). Soil respiration is implemented as an Arrhenius type equation (Lloyd and Taylor, 1994) in dependence of soil temperature in 7-12 cm depth. The used leaf area index (LAI) is monthly Moderate Resolution Imaging Spectroradiometer (MODIS) data, averaged for the years 2001-2010.
To improve the modeling of the passive tracer CO_2 a new advection scheme and its adjoint, the absolute monotone Walcek scheme (Walcek, 2000) has been implemented in the EURAD-IM. This prevents spurious wiggles occurring at sharp spatial CO_2 concentration gradients (e.g. close to strong anthropogenic point sources). Further problems occur if a non-monotone advection scheme is used in the presence of sharp spatial wind gradients in higher model layers, see Fig. 5.

Identical twin experiments are executed in two configurations with disturbed initial values and disturbed flux factors. Initial values are disturbed by 2 ppm, which can be easily exceeded by night-time transport (Gerbig et al., 2008). Flux factors for anthropogenic emissions, photosynthesis, and soil respiration are disturbed to 0.8 from the background value 1.0. The assimilation window is 12 hours from 06-18 UTC 23 July 2012. Artificial observations are taken at seven stations every 30 minutes as shown in Fig. 6. In experiment 1 only the flux factors are optimized, in experiment 2 additionally the initial state is optimized. Fig. 6 shows the benefit of joint optimization compared to an adjustment of fluxes only. Sole flux optimization overestimates biogenic fluxes in large areas, as observations at early times result in a too strong forcing of photosynthesis, increasing also biogenic respiration due to later observations. In the area of the observation stations Jülich and Selhausen, biogenic respiration is also underestimated, a clear deterioration of analysis performance compared to the joint analysis.

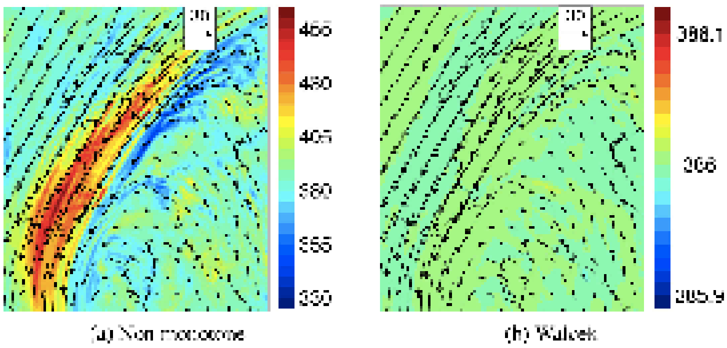

Figure 5: CO_2 mixing ratio at 320 hPa after 4 hours simulation, started with constant mixing ratio. Left: non-monotone advection scheme, right: Walcek advection scheme. The horizontal wind field is normalized to 30 m/s and has a strong spatial gradient between Po valley and the western Alps.

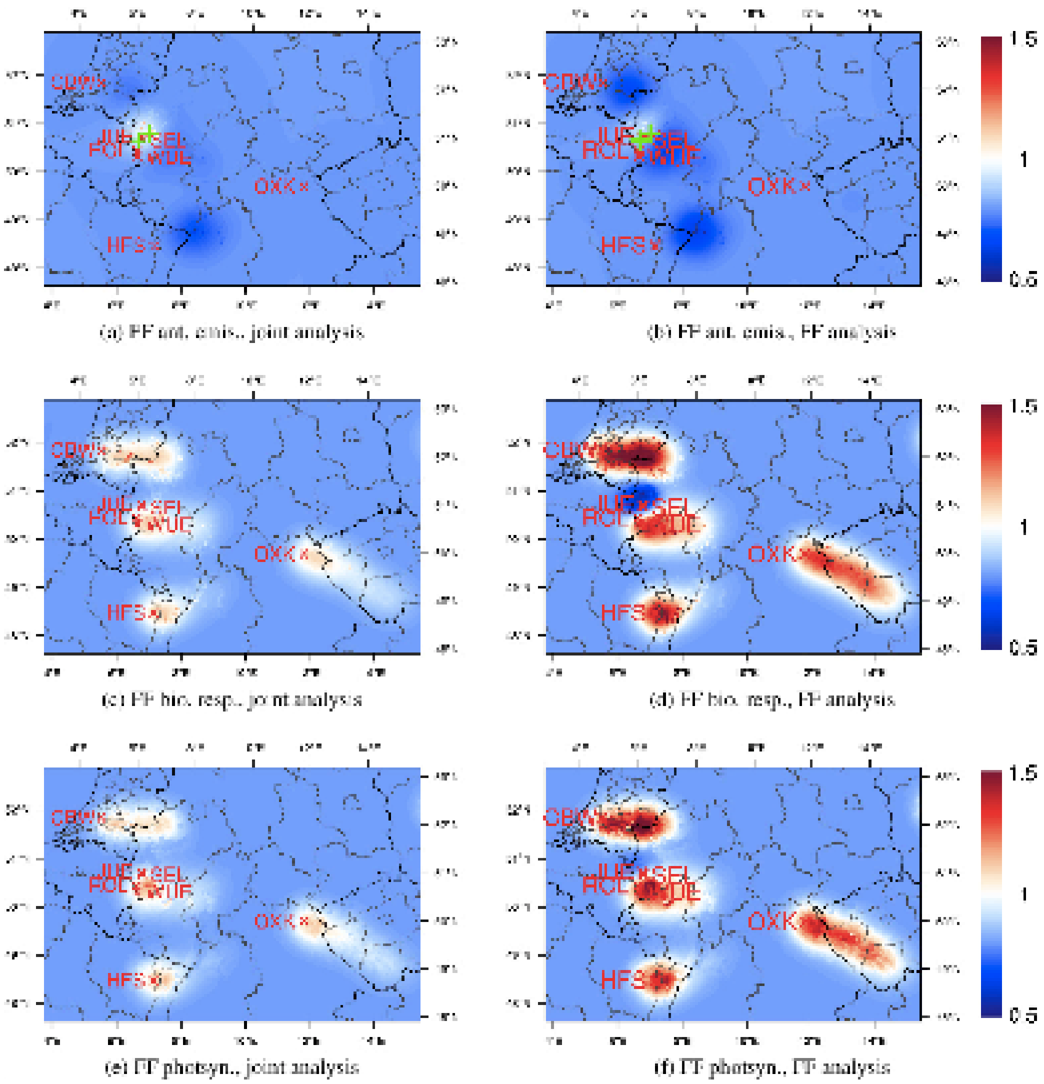

Figure 6: Analysed CO_2 flux factors. Above: anthropogenic emission fluxes, middle: biogenic respiration, below: photosynthesis. The left column shows results of the joint initial value and flux factor assimilation, the right column shows results of flux factor optimization an analysis which optimized only. The biogenic fluxes are shown at the surface level, while the anthropogenic emission fluxes are given at layer 6, which is the layer with the highest impact of power plants. Green plus signs indicate the location of the two biggest power plants Niederaußem and Weisweiler.

1.2 Volcanic emission data assimilation

To improve volcanic ash and gas emission dispersion forecasts, we performed a multidimensional (2D/3D) variational data assimilation study, using vertically highly resolved lidar (light detection and ranging) observations from NASA's CALIPSO satellite. Therefore, we developed a corresponding observation operator that maps the modeled quantity into the observation space. This includes in detail a look-up-table approach whereas the radiative transfer of the lidar signal is simulated based on Mie-theory (Fast et al., 2006; Wiscombe, 1980) and the lidar equation according to Huneeus u. Boucher [2007]. A case study regarding the ash cloud of the Eyjafjallajökull eruption in April 2010 over Western Europe is accomplished, discussed, and published in Wilkins et al. 2016 (see Fig. 12).

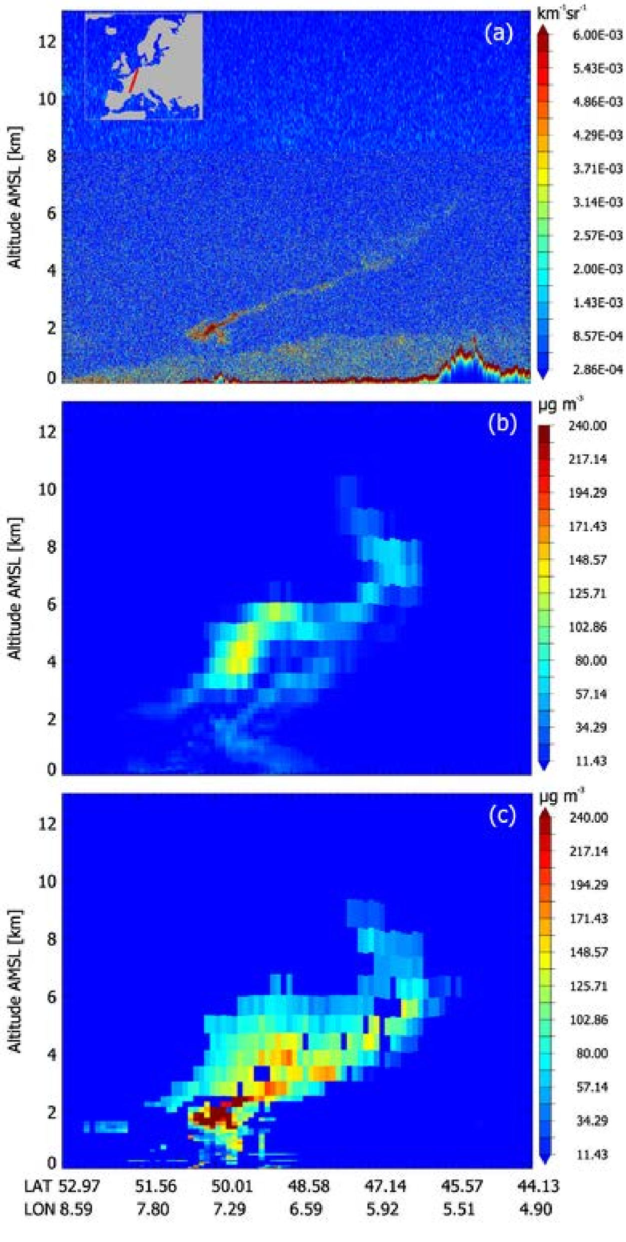

Figure 12: (a) Vertical cross section of the CALIOP total attenuated backscatter signal (532 nm) on 17th April 2010, on its flight path indicated in the European map in the upper left corner. (b) Vertical cross section of the a priori volcanic ash concentration by EURAD-IM for the same time and location as in (a). (c) Analysis of the volcanic ash concentration corresponding to the observations (a) and the a priori concentrations.

Further research activities are related to the last eruption of the Bardarbunga/Iceland (Aug. 2014 to Feb. 2015), which was characterized by a strong release of SO_2 into the lower troposphere while ash emissions were negligible. Hence, we aim to assimilate SO_2 concentrations in terms of vertical column densities observed by polar orbiting satellites such as GOME-2 and OMI. As a first case study a particular episode (Sep. 2014) with extremely high SO_2 concentrations recorded at several European measurement sides at ground level is considered. EURAD-IM is able to predict these high concentrations quite accurately looking upon forward simulations with roughly estimated emission parameters. Furthermore, the forecast results indicate that the unusual high SO_2 values, which were recorded at several European stations, are due to the transport of SO_2 rich air from Holuhraun towards continental Europe. However simulated concentrations stay in many cases below measurements of ground stations. The application of the EURAD-IM 4D-var system based on satellite observed SO_2 concentrations is required to improve these results.

2. Operational Ensemble Air-Quality Forecasts and Analyses for Europe

2.1 Air-quality forecasts

This task corresponds to the 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 are forecasts of O_3, NO, NO_2, SO_2, CO, NH_3, NMVOC, total PAN, $PM_{2.5}$, $PM_{10,}$ and birch pollen at the surface level and at 50, 250, 500, 1000, 2000, 3000, and 5000 m height. Recently the forecast products have been amended by olive and grass pollen number concentration.

2.2 Air-quality analyses

This task corresponds to the operational provision of hourly analyses for key air-quality compounds (O_3, NO, NO_2, SO_2, CO, $PM_{2.5}$, and PM_{10}) at the surface with EURAD-IM. Currently assimilated are situ observations from the EEA, OMI and GOME-2 NO_2 column retrievals, and MOPITT CO profile retrievals. Concentrations of NH_3, NMVOC, and total PAN are additionally provided although these components are not directly assimilated. A second analysis of the previous is performed in the early morning with a reduced set of observations to provide improved initial values for the subsequent forecast.

3. Validated Assessments of Air Quality for Europe

Main Objective of this sub-project is the yearly provision of air quality assessment reports based on validated ensemble re-analyses of the European air quality. 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.

Some constrains related to the availability of validated regulatory observation data from the EAA, appeared to be an issue for the publication of air quality assessment reports within a period shorter than two years. CAMS additionally aim at the provision of interim re-analysis reports based on un-validated surface observations. These reports will be delivered with a relatively short delay of a few months only.

The CAMS validated assessment reports are based upon an ensemble of models hosted at seven institutions in Europe, including RIUUK. During the accounting period the 2013 air quality re-analysis and the 2015 interim re-analysis were 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, and PM_{10} concentrations averaged over all Airbase background measurement sites, which were held back from assimilation for the year 2013.

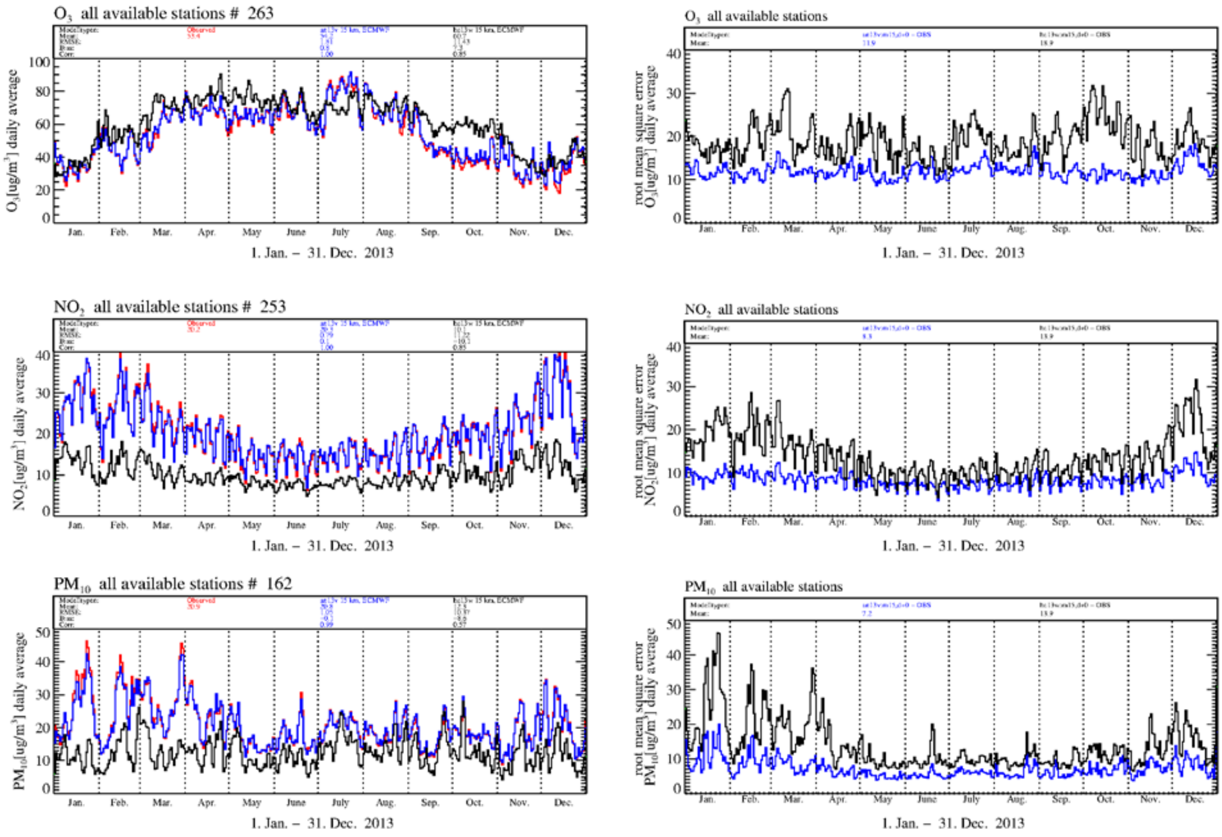

Figure 9: Daily averaged concentration (left) and its root mean square error (right) of O_3 (first row), NO_2 (second row), and PM_{10} (last row) averaged over all surface in situ measurement sites, which were held back from assimilation for the year 2013. Red: observations, blue: EURAD-IM 3d-var re-analysis, 30% of stations held back from assimilation, black: control run (no data assimilation at all).

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Summary of plans for the continuation of the project

The operational CAMS air quality forecast with the EURAD-IM model will be continued in the next reporting period. To improve the forecast quality in case of special events like Sahara dust outbreaks or volcanic eruptions, it is planned to add MODIS NRT AOD retrievals and satellite observations of SO_2 columns to the operational assimilation chain. An air quality re-analysis for the year 2014 and an interim re-analysis for the year 2016 will be performed with the EURAD-IM model to support the corresponding CAMS air quality assessment reports for Europe.