REQUEST FOR A SPECIAL PROJECT 2013–2015

MEMBER STATE: Germany

Principal Investigator[1]**:** Hendrik Elbern

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

Address: Aachener Str. 209
D-50931 Köln

Germany

E-mail: he@eurad.uni-koeln.de

Other researchers: Elmar Friese

Project Title: Monitoring Atmospheric Climate and Composition - Interim Implementation (MACC-II)

If this is a continuation of an existing project, please state the computer project account assigned previously.	**SP** DEFRIU

Starting year: (Each project will have a well defined duration, up to a maximum of 3 years, agreed at the beginning of the project.)		
Would you accept support for 1 year only, if necessary?	YES	NO

Computer resources required for 2013-2015: (The maximum project duration is 3 years, therefore a continuation project cannot request resources for 2015.)	**2013**	**2014**	**2015**
High Performance Computing Facility (units)	2370000	2370000	2370000
Data storage capacity (total archive volume) (gigabytes)	14600	14600	14600

*An electronic copy of this form **must be sent** via e-mail to:* *special_projects@ecmwf.int*

[1] The Principal Investigator will act as contact person for this Special Project and, in particular, will be asked to register the project, provide an annual progress report of the project's activities, etc.

Electronic copy of the form sent on (please specify date):

29.04.2012

Continue overleaf

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Extended abstract

Preliminary remark:

Regional Air Quality modelling in MACC-II is based on an ensemble approch. Aim of this special project is to develop and operate the EURopean Air pollution Dispersion – Inverse Model (EURAD-IM) as element of the regional ensemble. Compute resources are requested at ECMWF, because super computer at Research Centre Jülich are using job scheduling schemes, which do not grant regular day time dependent launch of jobs. There, queued jobs are executed without priority of submission schedules which are dependent of exact times of day, as indispendable for forecasting schedules. However, for achieving utmost operational stability a backup system will be installed at Research Centre Jülich during MACC-II.

Motivation:

The Proposal of MACC-II (Monitoring Atmospheric Composition and Climate – Interim Implementation) is an interim stage in the development of the GMES Atmosphere Service. Its overall institutional objective is to function as the bridge between the developmental precursor project MACC and the Atmosphere Service envisaged to form part of GMES Operations for 2014-2020. MACC-II will provide continuity and refinement of the atmospheric services provided by MACC. In addition, MACC-II will respond promptly when needed to supply specific products related to major events involving atmospheric constituents such as volcanic ash and pollutants from major fires, especially in cases of particular importance to the area of the European Union.

The scientific plan of this special project is fully based on the corresponding concept of MACC II, as it is detailed below for the individual work elements, and the Description of Work in more comprehensive terms. The assesment of the computer resources claimed as a conservative estimate of the operational needs, based on the experiences made in GEMS and MACC. As mentioned above, all computations outside the diurnal assimilation and forecasting schedule (except final preoperational tests) are separated and performed on RIUUK's and Research Centre Jülich's facilities.

The Rhenish Institute for Environmental Research is leader of sub-project 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-II.

RIUUKs model in the EURAD-IM, which is controlled by SMS software on ECMWF's compute platforms. This proved to be a stable and efficient set-up during the recent period.

1. Data Assimilation for European Air Quality (EDA)

EDA's principal objective is to assure increasing and skilful use of new trace gas and aerosol measurements or retrievals, within a scenario of changing earth observation data compositions, retrieval versions and model configurations, hence building on developments of R-EDA in MACC . These developments will be provided for prototype operational use in MACC-II sub-projects ENS and EVA.

While in MACC R-EDA activities laid the foundations for prototype operational chemical data assimilation procedures, with primary focus on *in situ* data, this proposal aims to (i) improve the regional DA system with respect to an extended or partly novel set of remote sensing data and *in situ* observations, (ii) generalize and refine the core data assimilation capacities of individual air-quality models in terms of operational stability, accuracy, and reliability, (iii) validate the assimilation system with refined methods and algorithms, and (iv) provide for validity of the data assimilation in case of extraordinary geophysical or atmospheric events.

The organization of work follows the four identified objectives, and is detailed below.

EDA 1 Satellite data assimilation

Satellite data for the troposphere will be prepared for prototype operational and case study use in data assimilation, with emphasis on efficient data processing, applying most recent error estimates from retrievals and balancing with *in situ* data. The character of most of this work is "Adaption of the service chain to new input data".

Basically it is the establishment of an extended suite of data to be assimilated from **space-borne sensors**:

- IASI data assimilation module for ozone
- MODIS, MSG/SEVIRI AOD data assimilation module

In addition, further ingestion of *in situ* data is planned. These are collected by EEA EIONET, comprising constituents under EU directive rule, including particulate matters in the limits of PM10 and PM2.5 and IAGOS-ERI aircraft data, which provide profiles over some major European cities.

EDA2 Assimilation algorithm extension

This work package introduces a couple of improvements of the assimilation algorithm, which will substantially extend its applicability, while improving robustness, and stability. The work is made in the frame of "Making minor improvements to existing production systems to maintain performance".

EDA.2.1 Aerosol data assimilation

The aerosol data assimilation is either introduced or refined to address the following issues:

- Observation-minus-model differences in AOD will be adjusted not simply by a suitable factor applied to all components. Rather, the adjustment is introduced according to the height dependent forecast error variances.

- Regularization of the aerosol components is introduced by a constraining function to assure realistic portions of aerosol components.

EDA.2.2 Bias correction scheme

The bias correction scheme will account for typical time-dependent model biases as found by EVA and

ENS evaluation.

EDA.2.3 Dynamic covariance evolution
This work task focuses on the optimal exploitation of background/forecast information from ensemble runs and the related formulation as covariance. The forecast/background error covariance matrix will be made flow dependent. This is done either by application of the "NMC"-method or by exploitation of the ENS model ensemble.

EDA.2.4 4d-var emission inversion
The emission data inversion procedure based on the 4d-var will be applied to identify emission correction factors. Emission factors to be improved comprise observed species in the first place, but also not observed, yet influenced by chemical coupling. The continued inversion of the model with respect to emissions should provide emission factors, which are able to improve forecast quality even in a free model run.

EDA.3 A posteriori validation
A posteriori validation is the means in data assimilation, to evaluate the skill of results in terms of data assimilation related algorithms. It tests the BLUE (Best Linear Unbiased Estimate) properties by means of consistency of results. The basic key approach is χ^2-validation, which enables the consistency test as a necessary condition. It cannot test the practical benefits in operation, which is left to sub-project ENS and EDA. The procedure is performed in two steps:

- Validation in terms of data available in near real time, and
- application of additional satellite data, which are not available in NRT, like IAGOS-ERI (as long as this is the case), or are not used like TES.

In all cases tests are also performed with data withheld from assimilation and used for validation.

EDA.4 Mineral dust, volcano and fire data assimilation
This work package comprises the development of measures to address data assimilation modifications for special transient atmospheric conditions. These include biomass burning, mineral dust events, and, based on recent experience in Europe due to the Eyjafjallajökull eruption, volcanic emissions. The data assimilation algorithm will be extended to identify the chemistry models' change toward local fire emsissions, estimate the forecast errors, adapt the covariance formulation, and perform the data assimilation procedure.

2. Ensemble Air-Quality Forecasts for Europe (ENS)
ENS primarily focuses on the delivery and verification of the prototype operational European-scale regional NRT air-quality services. In direct continuation from MACC, this service is based upon an ensemble of forecasts performed at seven centers in Europe, including RIUUK. The individual forecasts will use ECMWF operational meteorological forecast data, the regional air quality assimilation systems developed and tested within EDA, as well as the chemical boundary conditions provided by GDA. Every day, forecasts for each hour out to 96h ahead and analyses for the day before of key atmospheric pollutants in the form of maps and numerical data will be produced.

The main work packages in which RIUUK plays an active role are detailed below.

ENS.2 Model development including extension to CO_2 modeling
This work package corresponds to the continuous development of the Air Quality models involved in the regional core services (ENS and EDA). ENS.2 includes also a research component on Air Quality forecasting (process-oriented studies, developing and testing new ensemble methodologies...) and new developments on regional carbon dioxide modelling, in view of potential future high-resolution surface CO2 fluxes inversion products over Europe (which is beyond the scope of MACC-II). Such

supporting research and development activities are vital for maintaining GMES atmosphere regional products at the highest in international standards.
An important further development of the EURAD Air Quality forecast will be the inclusion of emission data from the global fire assimilation system (GFAS) developed by MACC-II sub-project FIR. On the MACC-II kick-off meeting EURAD-IM was selected as the pilot regional model for the application of GFAS data.

ENS.3 Air-quality forecasts
This task corresponds to the prototype operational provision of forecasts for key air-quality compounds with the seven individual model suites, which are developed and constantly updated within ENS.1. Forecasts, up to 96h (an extra 24h forecast compared to the situation in MACC is necessary to accommodate users' needs that require to have 72h of forecasts just after 00 UTC daily, in practice too early for the MACC-II ensemble forecast to be available) will be provided for a range of molecules and vertical levels in GRIB2 and netCDF format. Core product are forecasts of O_3, NO, NO_2, SO_2, $PM_{2.5}$, PM_{10}, CO at the surface level and at 500, 1000, and 3000 m height. These core products will be verified at the surface on a daily NRT basis. A further requirement of MACC-II users, especially from the FP7 project PASODOBLE, is to provide additional chemical species with an increased vertical resolution. This is necessary because the core products have been shown to be sufficient to apply as boundary values for down stream AQ simulations.

ENS.4 Pollen forecasts
This work package corresponds to the development of pollen forecast capabilities within the ENS regional core service.
Biogenic particulate matter (pollen grains, enzymes and other genetic material released by plants, spores, etc.) contributes significantly to primary particulate matter mass and affect its size distribution. Due to their seasonal character, they affect also the temporal variation of primary PM in the atmosphere. The introduction of primary biogenic PM as intrinsic component of particulate matter in Europe is expected to improve significantly the forecast of PM in the region. A pre-operational birch pollen forecast is scheduled at the end of 2013.

ENS.5 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, $PM_{2.5}$, PM_{10}, CO) with the seven assimilation suites (developed within EDA), including EURAD-IM. Hourly analyses for the previous day will be delivered daily. At first, this will be done once per day in the early morning with a reduced set of observations to provide improved initial values for the subsequent forecast. A second analysis for the previous day will be set up in the early afternoon, which includes as many as possible observations from all available NRT instruments.

ENS.8 Transition to operations
ENS.8 is a new component compared to MACC: It is aimed at specifically organizing the transition from prototype operational to fully operational services, which requires end-to-end analysis for the seven individual production lines and for central processing of the NRT regional core services for the atmosphere.
The first year of MACC-II will be devoted to the analysis of the existing procedures set up by the different regional partners: the 8 production chains (7 individual models, central processing and ENS platform) will be described in full detail, assessing the level of operationality of each step and the corresponding risks for failure. In particular, these activities will establish operationalization plans, compatible with the timing and resources of MACC-II.
The rest of the project will be devoted to the implementation of these operationalization plans, with the objective of being ready for full operational status at the end of MACC-II. During the last year, a task will study the opportunity of a certification (ISO9001) of the regional services, and document the steps and effort needed at each of the partners.

An adaption of the forecast scripts on ECMWF and Research Centre Jülich super computer is planned in order to improve stability and maintainability of these jobs. The different scripts have to be evaluated and modificated so that they melt into one basic script which can be used individually for each super computer system.

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

In MACC-II, the objectives of the EVA sub-project are the development and implementation of an operational process dedicated to the yearly production of European air quality assessment reports. These reports will be based on the MACC-II assimilation and modeling capacities, and will provide **the state and evolution of background concentrations of air pollutants in Europe, according to a number of indicators** relevant for policy use (regulatory indicators) and impact assessment (health and ecosystems exposure oriented).
Seven regional state-of-the-art compliant air quality models, including EURAD-IM, that run within the MACC-II prototype operational process and are proving their capacities and operationality, are involved in the service production. Each modeling team is responsible for upgrading model capacity and for the quality of the results this provides.
An increasing amount of available observation data is expected up to 2015, especially through the GMES *in situ* and satellite data coordination. The wealth of data currently available and expected in the near future should be considered in the operational products as they go along. Moreover, the continuous improvement of models and data-assimilation techniques (including ensemble approaches) will be taken into account for an overall improvement of the EVA products. Work to be done by each involved modeling team includes

- Assimilating new types of observational data in their reanalysis chain.
- Producing individual model re-analyses for the years 2011 to 2013.
- Evaluating model performance.

4. Justification of Computer Resources and Technical Description of Code

The system for the computational work to be done in the work packages of MACC-II is the EURAD-IM model system. This model system consists of 5 major parts: the meteorological driver WRF, the pre-processors EEP and PREP for preparation of anthropogenic emission data and observations, the EURAD-IM Emission Model EEM, and the chemistry transport model EURAD-IM. The data flow of the EURAD-IM system is depicted in Figure 1. EURAD-IM is a meso-scale chemistry transport model involving transport, diffusion, chemical transformation, wet and dry deposition and sedimentation of tropospheric trace gases and aerosols. It includes 3d-var and 4d-var chemical data assimilation and is able to run in nesting mode.

On ECMWF's compute server c1a, the EURAD-IM uses 121 CPU's with are parallelised with MPI. The new installed Weather Research & Forecasting Model (WRF) will also be parallelized with MPI using 120 CPU's.

The Supervisor Monitor Scheduler (SMS) is used to control the pre-operational air quality forecast as well as the analysis of the air quality of the previous day.

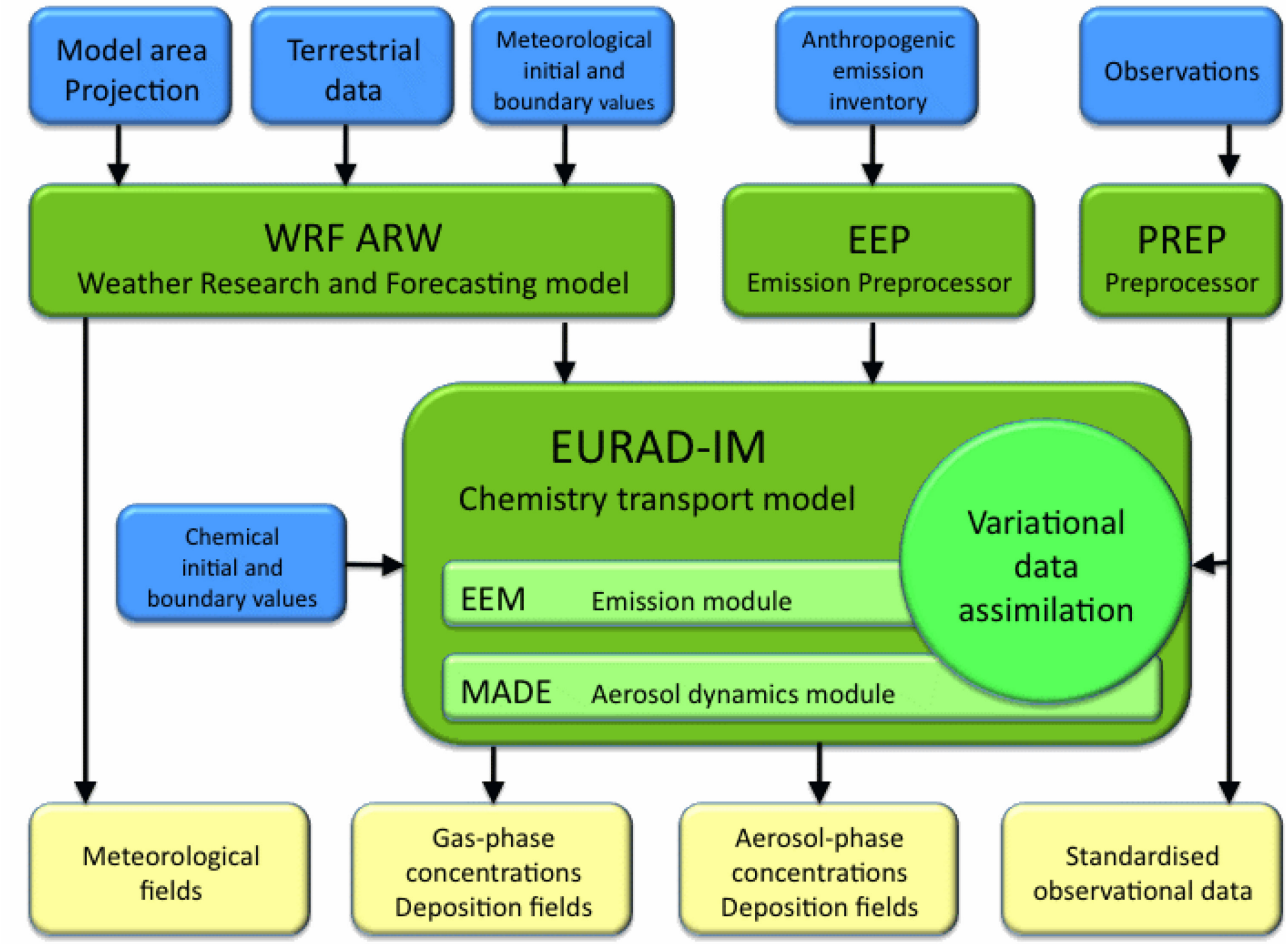

Figure 1: Flowchart of the EURAD-IM model system containing the meteorological driver WRF, the pre-processors EEP and PREP, the emission model EEM and the chemistry transport model EURAD-IM (input parameters are shaded in blue, output parameters are shaded in yellow and procedural parts are shaded in green).

Computer resources requested are mainly due to the following work packages:

ENS.3 Air quality forecasts

The pre-operational air quality forecast for Europe, based upon the 12:00 IFS operational meteorological forecast, has been set up using the continental-to-local scale chemical data assimilation system EURAD-IM with 15 km resolution. A 96h forecast of O_3, NO, NO_2, CO, SO_2, $PM_{2.5}$, and PM_{10} is regularly delivered. Chemical initial and boundary values are provided by the pre-operational 3d-var analysis for the previous day and MACC-II sub-project GDA, respectively. Computing resources needed are 1290 SBU's per day for the meteorological driver WRF and about 3100 SBU's per day for the chemistry transport model EURAD-IM. This results in an amount of about 1,600 kSBU's per year.

ENS.5 Air quality analyses

Using the system developed and tested within sub-project EDA, daily pre-operational 3d-var air quality analyses based upon the 00:00 IFS operational forecast are provided for Europe with 15 km resolution. For this purpose near real time surface in-situ measurements of O_3, NO_2, NO, SO_2, CO, and PM_{10} as well as satellite derived NO_2 column retrievals from OMI, GOME-2, and SCIAMACHY

are hourly assimilated using the intermittent 3d-var method. This task needs about 210 SBU's per day for the meteorological driver WRF and about 1,300 SBU's per day for the chemistry transport model EURAD-IM, which results in an amount of about 550 kSBU's per year.

About 2150 kSBU's per year are probably sufficient to fulfill the requirements of sub-projects R-ENS ans R-EVA. An overhead of about 10 % is expected to be necessary to test new developments.