

# SPECIAL PROJECT PROGRESS REPORT

**Reporting year** 2008/2009

**Project Title:** GEMS: Global and Regional Earth-System Monitoring using Satellite and in situ data  
Work Package WP RAQ 2  
MACC: Monitoring Atmospheric Composition and Climate

**Computer Project Account:** SP DEFRIU

**Principal Investigator(s):** Hendrik Elbern

**Affiliation:** Rhenish Institute for Environmental Research at the University of Cologne, RIU (FRIUUK)

**Name of ECMWF scientist(s) collaborating to the project (if applicable)** Dr. Adrian Simmons

**Start date of the project:** GEMS: March 2005, MACC: June 2009

**Expected end date:** GEMS: May 2009, MACC: late 2011

**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
<b>High Performance Computing Facility</b>	(units)	100,000	98,000	1,700,000	1,010,000
<b>Data storage capacity</b>	(Gbytes)	750	900	10,000	6,400

## Summary of project objectives

Project work is exclusively restricted to the FRIUUK contribution to the work packages WP\_RAQ2, WP\_RAQ4, and WP\_RAQ5 of GEMS and to the work packages R-EDA, R-ENS, and R-EVA of MACC. The continental-to-local scale chemical data assimilation EURAD-IM system with both its full 4d-var and 3d-var assimilation options is implemented. The system operates to perform the tasks invoked by GEMS and MACC for FRIUUK. The tasks include development and delivery of improved data assimilation methods to assure optimal exploitation of observations, assimilation of available data from both in situ and satellite devices, provision of pre-operational NRT daily air quality forecasts, and performance of regional air quality hindcasts over the year 2003. The lateral boundaries of the EURAD-IM model domain will be coupled with the global chemistry transport models MOZART, TM5, and MOCAGE.

## Summary of problems encountered

The computer resources allocated for the year 2009 are not sufficient to run the EURAD-IM pre-operational air quality forecast with the resolution of 15 km over the whole year to comply with GEMS RAQ plannings. The cause of this is that air quality hindcasts over the whole year 2003, which were performed to achieve the requirements of GEMS WP RAQ5, consumed more computing resources as expected. Current estimates indicate that about 100 kSBUs more as requested are needed for the year 2009. Domestic compute capacities are occupied by other projects and insufficient. Research Centre Jülich compute capacities are accessible but can be used for non time-critical applications only. Queuing regulations at the Research Centre circumvent a forecast that is finished according to schedule. Waiting times more than a day are frequently experienced.

## Summary of results of the current year

(from July of previous year to June of current year)

A 3d-var air quality analysis system has been developed and is running re-operational at ECMWF since mid of September 2008. The analysis system consists of three components: the meteorological model MM5, an observation data pre-processor, and the inverse modelling version of the EURAD CTM (EURAD-IM). The IFS 00:00 UTC forecast is used to provide initial and boundary values for the MM5. Between 23:00 UTC and 00:40 UTC the observation data pre-processor is running to prepare in situ-data from France and the Federal Environment Agency (UBA) as well as OMI, GOME-2, and SCIAMACHY NO<sub>2</sub> tropospheric columns for the subsequent assimilation procedure. At 24 times during the day the observations within a one hour interval are assimilated using the intermittent 3d-var method. A 24 hours analysis of the previous day is available at about 01:00 UTC. The analysed model state at midnight is used as initial model state for the subsequent 72 hours air quality forecast.

Mid of February 2009 the horizontal resolution of the 3d-var analysis system has been increased from 45 km to 15 km. The significantly increased CPU time requirement forced a broadening of the assimilation window from one hour up to three hours, which means that observations are assimilated at eight times during a day in the current configuration.

The impact of chemical initial values originating from the 3d-var analysis on the forecast quality has been studied for the period 16th of September to 22th of September 2008. Horizontal model resolution for this experiment has been set to 45 km. Concentrations of O<sub>3</sub>, NO<sub>2</sub>, SO<sub>2</sub>, and CO derived first from a free forecast initialized with the model state D+1 of the free forecast from the previous day, and second derived from a free forecast initialized with the final model state of the 3d-var analysis of the previous day are compared with hourly measurements at all available stations from the Federal Environment Agency (UBA). Figure 1 show time-series of spatially and temporal averaged concentrations of O<sub>3</sub> and SO<sub>2</sub>. After six hours the impact of data assimilation on the forecast quality of O<sub>3</sub> is insignificant due to advection of air masses which were not subject of the assimilation procedure as well as due to fast chemical reactions. The influence of chemical reactions can not be covered by initial values derived from a 3d-var analysis. In case of the low reactive species sulphur dioxide the impact of data assimilation on the forecast quality is significant during the first 12 hours at least.

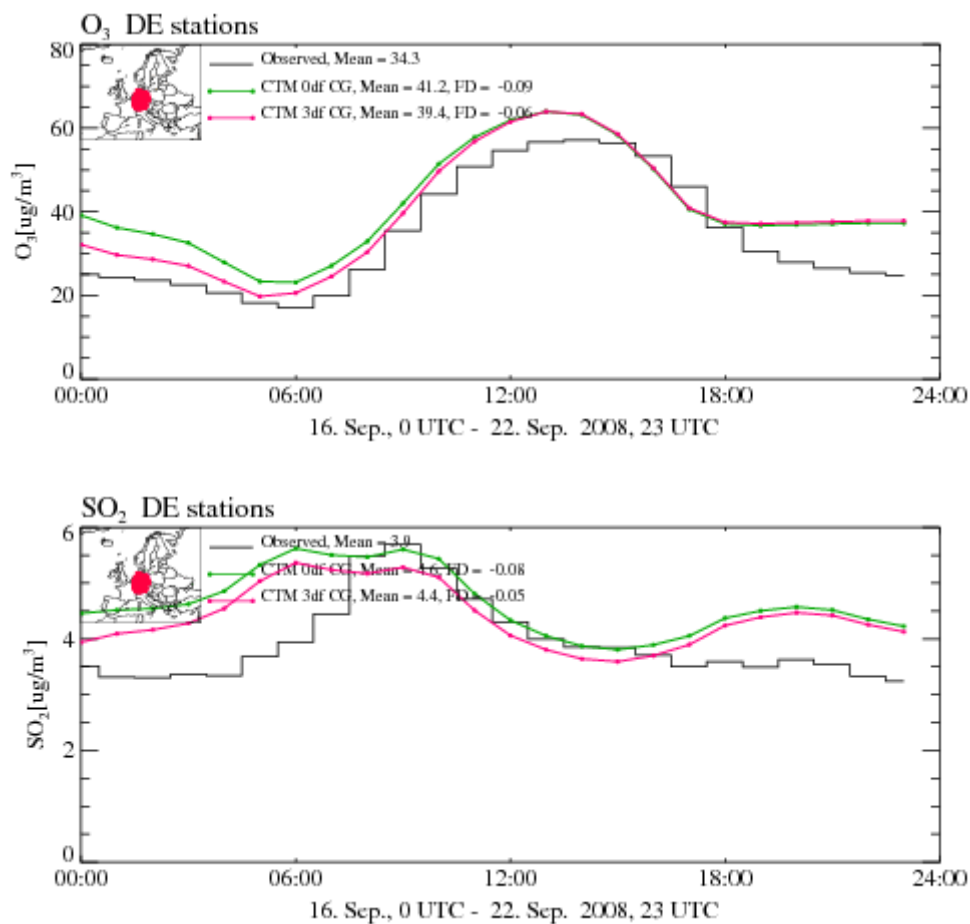


Figure 1: Hourly O<sub>3</sub> (above) and NO<sub>2</sub> (below) concentrations averaged over the period from 16<sup>th</sup> to 22<sup>th</sup> of September 2008 averaged at all available stations from the Federal Environment Agency (UBA). Green: Model results from a free forecast initialized with the model state D+1 of the forecast from the previous day, red: model results from a free forecast initialized with the final model state of a 3d-var analysis of the previous day, black: measurements.

A 4D-Var experiment for European-scale tropospheric gas phase chemistry has been performed for the period July 2006. Both SCIAMACHY and OMI satellite retrievals from KNMI were assimilated by averaging kernels, using error information from the data provider. In an attempt to provide a horizontal model resolution comparable to the minimal OMI 24x13 km<sup>2</sup> footprint, the model resolution was set to 15 km. The Data assimilation configuration has a time window of three hours (09:00-12:00 UTC) to include Envisat satellite data with a late morning overpass over Europe and OMI overpass in early afternoon over Eastern Europe. After assimilation, a 24-h forecast is made, starting at 08:00 UTC; the analysis produced by the assimilation is the initial field, and an emission rate correction factor is applied. A clear validation result indicating forecast skill improvements by surface in situ stations is hard to obtain. On the one hand the averaging kernel with only 10% average signal strengths at the ground implies only minor impact in near surface layers, while on the other hand NO<sub>2</sub> is reacting too fast for displaying a direct benefit for the next days forecast. As concerned the indirect effect via ozone improvement, two cases must be distinguished: In the rural case, ozone formation is often controlled by low NO<sub>x</sub> levels, where the signal/noise ratio is unfavourable and assimilation impact is low. In the case of urban areas, the spatial resolution problem of the model and its emissions prevail.

As preparation of the air quality hindcast over the GEMS re-analysis period the periods from 1<sup>st</sup> of January to 6<sup>th</sup> of April 2003 and from 1<sup>st</sup> of July to end of September 2003 respectively have been simulated with 25 km resolution. Over prediction of gaseous (NO<sub>2</sub>, SO<sub>2</sub>, NH<sub>3</sub>) and particulate (NO<sub>3</sub><sup>-</sup>, NH<sub>4</sub><sup>+</sup>) constituents during the winter episode caused some further development of the EURAD-IM CTM. The gas-phase dry deposition parameterization according to Wesely (1989) has been replaced by a method used within the AURAMS model (Zhang et al., 2003). Calculation of inorganic aerosol thermodynamics is now based on a new temperature dependent parameterization of the Pitzer, Simonson, Clegg (PSC) ion interaction model for the system NH<sub>4</sub><sup>+</sup>, NO<sub>3</sub><sup>-</sup>, SO<sub>4</sub><sup>2-</sup>, H<sub>2</sub>O. Due to this modifications of the EURAD-IM CTM the model performance during the winter episode could be significantly improved. The impact on results for the summer episode is marginal, as desired.

An air quality hindcast for the whole year 2003 has been performed using the IFS re-analysis to provide initial and boundary values for the MM5 and taking the chemical boundary values from the global GRG and AER re-analyses. Volume mixing ratios of 15 chemical constituents with a time-step of three hours are provided by MOZART-IFS for the preparation of gas-phase boundary values. Concentrations of mineral dust (represented using three size bins), hydrophobic and hydrophilic organic matter, hydrophobic and hydrophilic black carbon, and sulphate from the global AER re-analysis are used to prepare boundary values of the EURAD-IM aerosol species mineral dust, organic carbon, elemental carbon, and sulphate with a time-step of six hours. Figure 2 show an example for the influence of boundary values from the AER re-analysis on the regional re-analysis for Europe. Intermittent 3d-var has been used to improve the quality of the hindcast. GOME NO<sub>2</sub> columns and O<sub>3</sub> profiles (first half of 2003), SCIAMACHY NO<sub>2</sub> columns (second half of 2003), EEA in situ data and MOZAIC measurements were assimilated each hour.

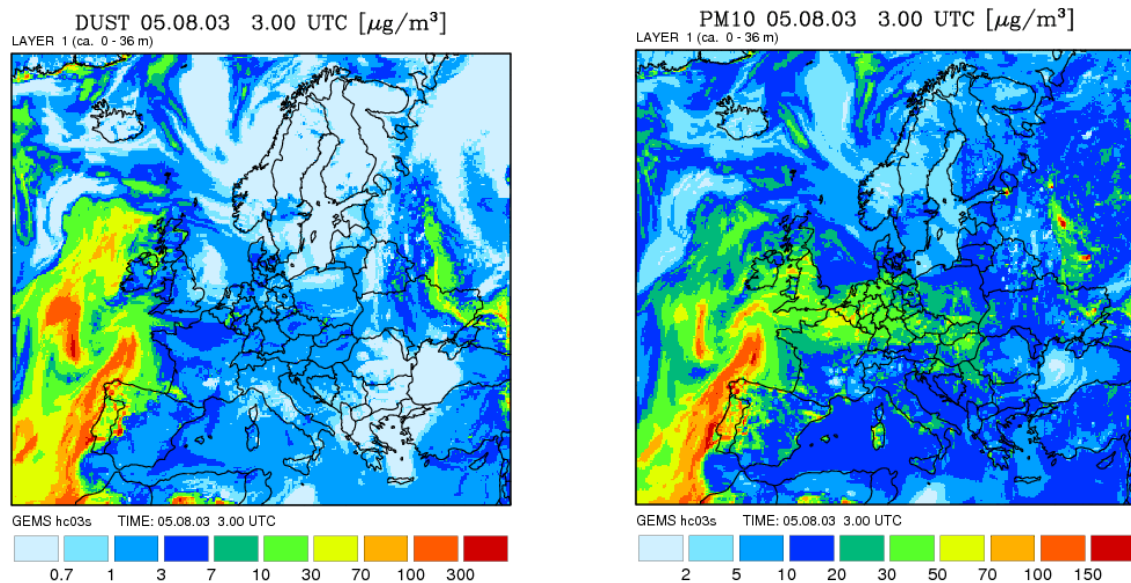


Figure 2: Mineral dust (left) and PM<sub>10</sub> (right) concentrations in the near-surface layer at 03:00 UTC of 5<sup>th</sup> of August 2003. High mineral dust concentrations over the south-west part of the model domain are caused by inflow through the lateral model boundaries. The AER re-analysis has been used to provide boundary values.

To investigate the impact that have time-dependent chemical boundary values (WP\_RAQ\_2.1), a second hindcast for the whole year 2003 has been performed using climatological boundary values. Monthly averages of the MOZART-IFS re-analysis, and the standard EURAD-IM climatological boundary values have been used for the gas-phase and aerosol-phase, respectively. To produce comparable results, the same data assimilation procedure as described above has been applied for this hindcast experiment.

A further hindcast has been conducted to cover the work planned for WP\_RAQ\_1.3. Covering the period from 1st to 15th of August 2003 the horizontal resolution of MM5 and of the EURAD-IM CTM has been increased from 45 km to 15 km. Boundary values from GRG/AER re-analyses are used for this hindcast experiment, and the data assimilation procedure applied is the same as that used for the experiments described above.

### List of publications/reports from the project with complete references

Hollingsworth, A. et al., The Global Earth-System Monitoring using Satellite and in situ data (GEMS) Project: Towards a monitoring and forecast system for atmospheric composition, Bulletin of the American Meteorological Society, 2008, DOI 10.1175/2008BAMS2355.1

## **Summary of plans for the continuation of the project**

Operation and improvement of the systems developed during GEMS is continuing in MACC. The tasks scheduled in MACC subproject R-EDA include provision of observation forward operators and its adjoint operators for various types of routine observations and retrievals, and related error covariances. Multi-model forecasts will be taken as basis information for the design of forecast background error covariance matrices, aiming to optimize the design toward anisotropic and inhomogeneous influence radii. In MACC subprojects R-ENS and R-EVA the air quality forecast system will be continued further developed and validated against surface in-situ measurements.