

# Updated and validated assimilation system specification for the production of operational air quality reanalyses

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This deliverable relates to the modelling and data assimilation chains that have been developed for the MACC/EVA service dedicated to the operational production of air quality assessment throughout Europe. Seven European modelling teams were involved in this subproject.

The MACC project demonstrated the feasibility and the relevance of such a system, but also its high level of ambition. A number of difficulties have been encountered by the modelling teams to run operationally data assimilation chains and to provide high quality results. However the outcome of this first phase of the GMES ATmopsheric Service is very positive and quick improvements are expected in the early stage of MACC2 (see the report on the MACC/EVA service ref D-R-EVA\_2.3).

To establish an in-depth and objective analysis of the situation concerning the EVA modelling systems when the MACC project finished, a questionnaire has been sent twice by INERIS to the MACC regional modelling teams: at the mid-term of the project, in September 2010 and at the end of the project in December 2011. This initiative helped to review and follow potential difficulties for setting up decentralised European air quality re-analyses chains and gathering their results in an ensemble product. It allows the evaluation of the gap between the actual modelling platforms that run for the provision of 2007-2008 and 2009 re-analyses and the future ideal system. With the MACC experiment, the specifications of such a system that will drive MACC2 developments can be established.

## 1 Specifications of the European air quality re-analysis system

### 1.1 General issues

Consistently with the infrastructure adopted for the air quality forecasts and near real time analyses production (ENS), the EVA air quality re-analyses platform is split in two parts:

- **The decentralised individual modelling systems which provide regional air quality simulations.** A number of input data is fixed and shared by all models: emissions, meteorology, boundary conditions. They are provided by the other MACC services (EMIS, FIRE, global subprojects) and by ECMWF for the meteorological re-analyses. The basic in-situ observation datasets used for data assimilation and performance evaluation respectively are predefined by the service coordination and not modified by the individual teams. However they are free to choose in available datasets research data and satellite retrievals that could improve their modelling systems or contribute to enhanced assessments.
- **The centralised modelling system provides ensemble re-analyses and realises evaluation of all model results.** It gathers all individual simulations and processes them following some QA/QC principles (projection of the results on the same grid, completeness checking, absurd values tracking...). The centralised system generates numerical maps of concentrations and various exposure indicators, according to the EVA reports needs and the users' requirements.

The following schemes (Figure 1 and Figure 2) summarise the regional air quality re-analysis system general specifications as they were set in MACC for the first stage of the air quality assessment service and as they should be in MACC2:

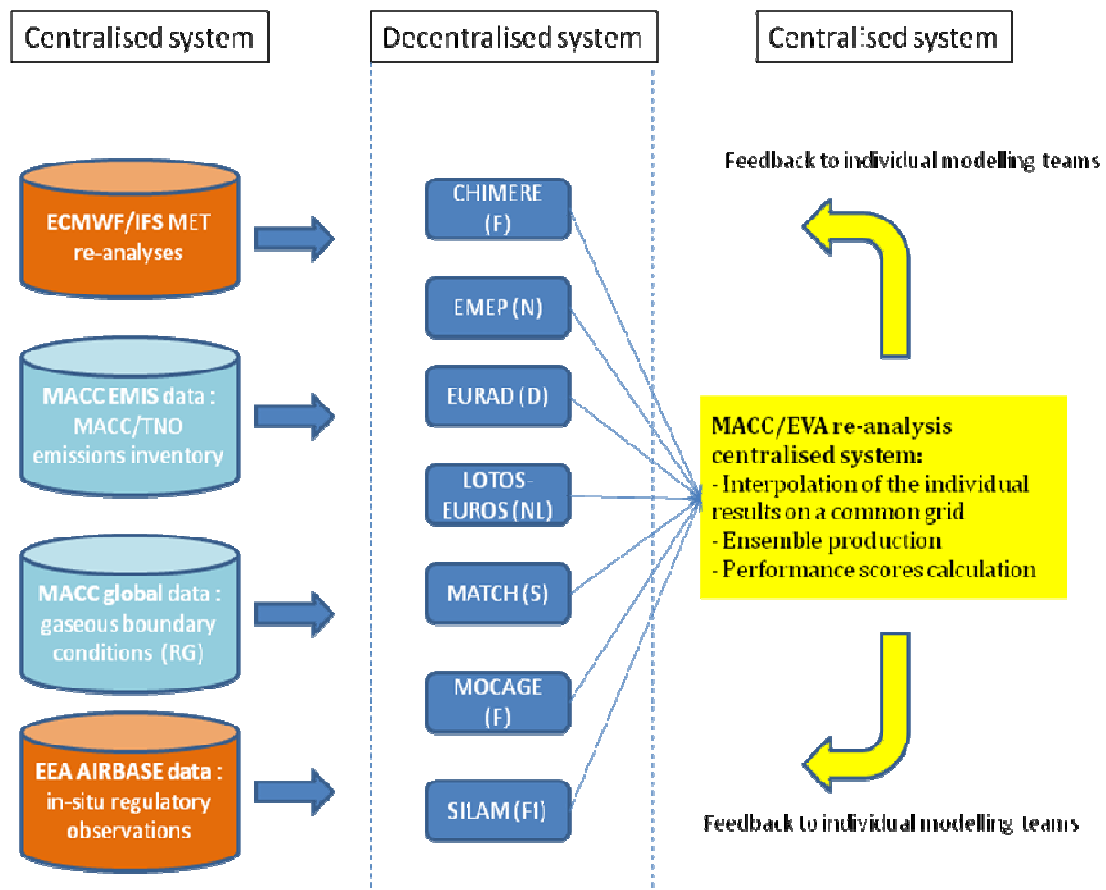


Figure 1. MACC/EVA system general specifications (as it runs for the 2007-2008-2009 productions)

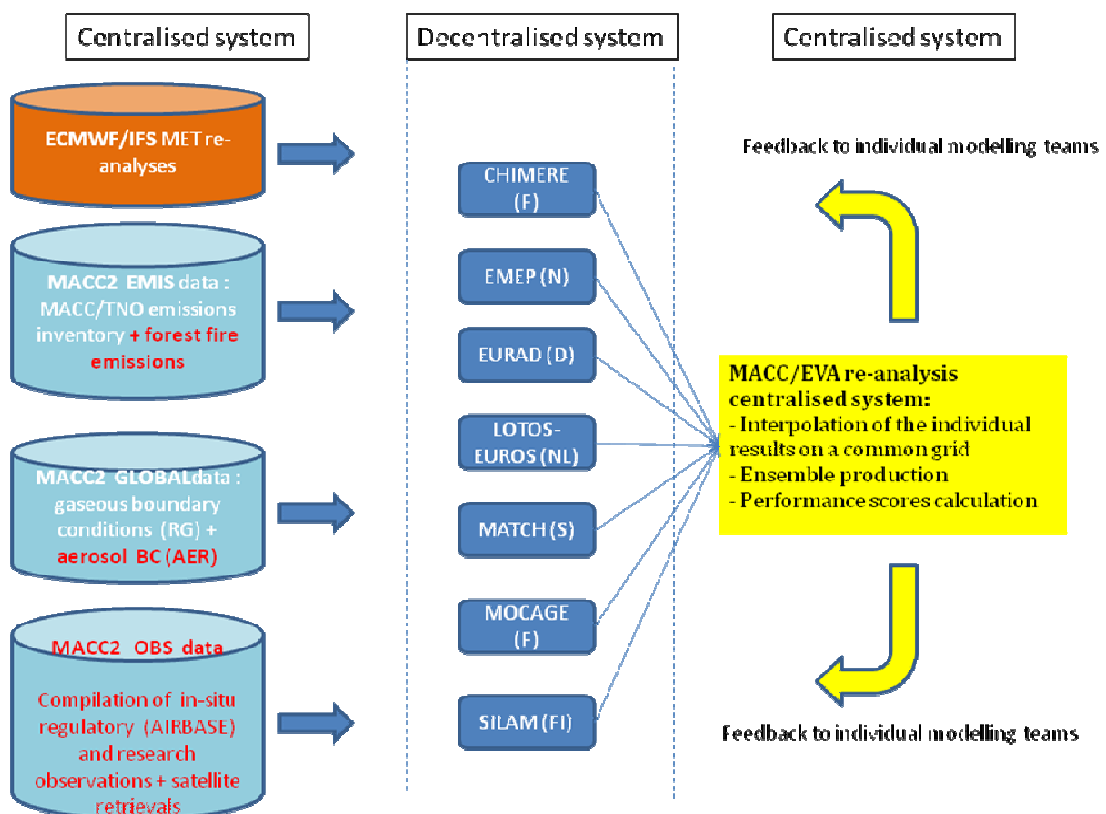


Figure 2. Future MACC2/EVA general specifications

## 1.2 The decentralised part

The “decentralised” part consists in the individual model chains that are developed in the MACC regional clusters. The models should be able to simulate transport and chemistry of atmospheric pollutants at the European scale to produce relevant concentration fields of ozone, PM and nitrogen dioxide.

The data assimilation chains are developed within the MACC/EDA subproject (MACC2/EDA in the future). Each team is free with the choice of the data assimilation strategy provided that the results are relevant, reliable and improve significantly the raw simulation results. Data assimilation strategy relates not only on the assimilation approach but on the choice of the assimilated data as well. The status of the data assimilation chains development for EVA operational purposes is described in the next paragraph.

Specifications for the decentralised regional modelling systems:

Characteristics	MACC specifications	MACC2 specifications
Domain	GEMS (Europe)	Extended domain to include Turkey and Island
Spatial Resolution	20-25 km	10km by the end of the process
Vertical domain (height, number of levels)	Free	Free
Emission data	TNO/MACC emission inventory (7km)	Improved MACC2 emission inventory + forest fires emissions
Boundary conditions	Gas: from MACC/GRG re-analyses (MOZART)	MACC2/GRG + MACC2/AER to include global aerosol products
Meteorological re-analyses	IFS (ECMWF)	IFS (ECMWF)
Chemical pollutants computed	O <sub>3</sub> , NO <sub>2</sub> , PM <sub>10</sub> , PM <sub>2.5</sub>	O <sub>3</sub> , NO <sub>2</sub> , PM <sub>10</sub> , PM <sub>2.5</sub> , SO <sub>2</sub> , C <sub>6</sub> H <sub>6</sub> To match with the AQ Directives, feasibility for heavy metals and PAHs will be considered
Chemical schemes	Free	Free
Pollutants from natural sources	Experiment with SILAM to assess the feasibility of pollen assessments	Pollen operational Dusts included (with MACC2/AER inputs) Feasibility for volcanoes eruption events
Data assimilation approach	Free	Free
In-situ data	AIRBASE observations +	AIRBASE (mandatory) Extension of the in-situ network to research networks
Earth Observations	experiments with satellite observations (RIUKK, KNMI)	Assimilating Earth Observations becomes mandatory ... Observation sets will be discussed
Accuracy	Consistent with the AQ Directive requirements: difference between hourly modelled and observed data should not exceed 50%	Criteria will be set following the FAIRMODE group recommendations ( <a href="http://fairmode.ew.eea.europa.eu/">http://fairmode.ew.eea.europa.eu/</a> )

### 1.3 Centralised system

INERIS as the coordinator of the sub-project EVA is responsible for the development and the implementation of the centralised core system which produce final EVA assessments: maps, exposure indicators, statistics, and performance scores.

The centralised system should allow the generation of specific maps and graphs to be systematically presented in the assessment reports.

The sets of observation data to be used for a given year should be prepared at the centralised level too and distributed to the modelling teams so that common information on observation data used both for assimilation and for validation could be shared.

Within MACC, the centralised part functionalities have been discussed among the modelling teams thanks to informal meetings and e-mail exchanges. In MACC2 a more formal organisation will be set up, based on a steering Committee. A representative of each modelling team will participate to this Committee that will act as an editorial committee when the content of the assessment reports will be decided and reviewed. Figure 3 below synthesises the functionalities of the centralised part managed by INERIS with fluxes towards and from the decentralised modelling teams. The future Steering Committee will yearly review the products and the process. Figure 4 shows in details the ideal cycle that should drive the EVA assessment report production. This concept is issued from the MACC experience considering realistically the time needed to get and process observation data and for iterating with the individual modelling teams on their model results. Actually in MACC this cycle has not been respected because the individual modelling systems were still under development or in their validation phase. It is expected that it will be possible to implement it in MACC2 for the 2010 assessment report production.

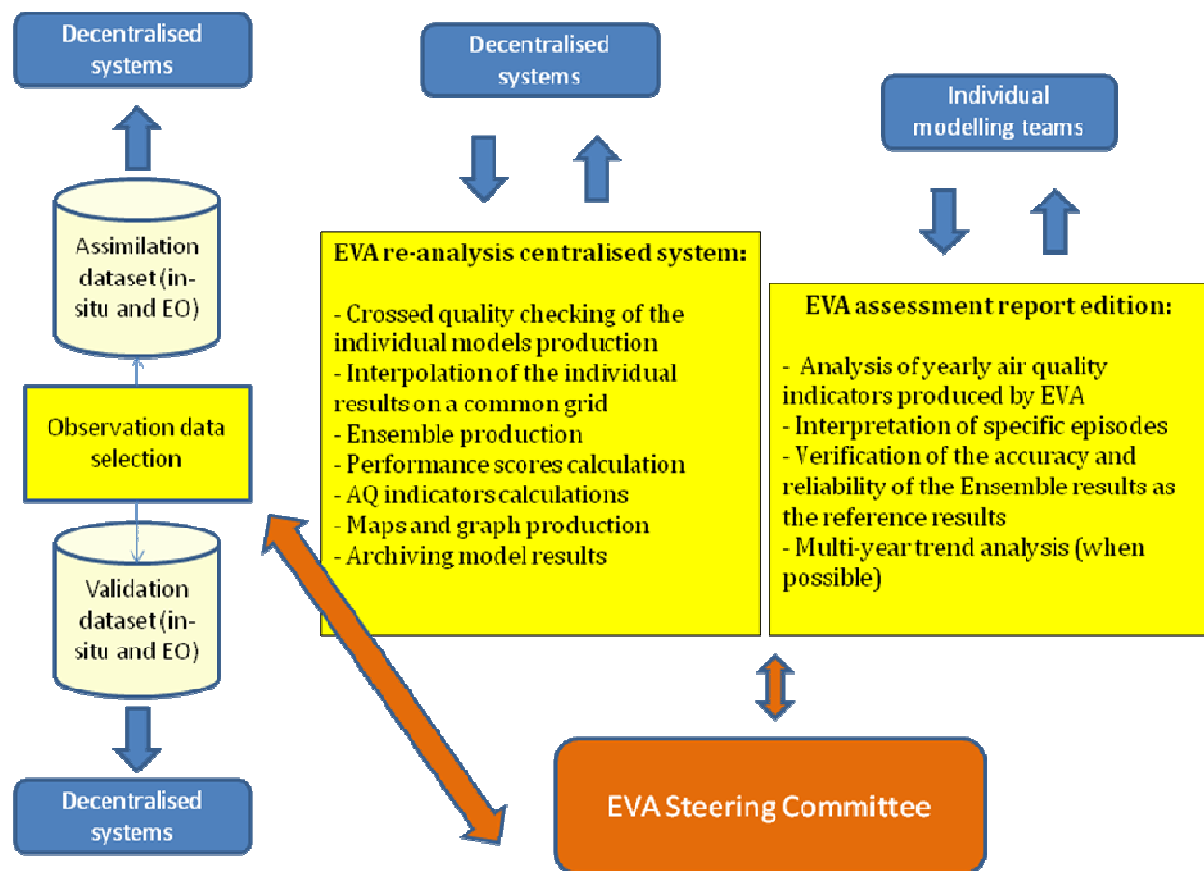


Figure 3. Organisation of the centralised part of the EVA sub-project and links with the decentralised parts and the Steering Committee

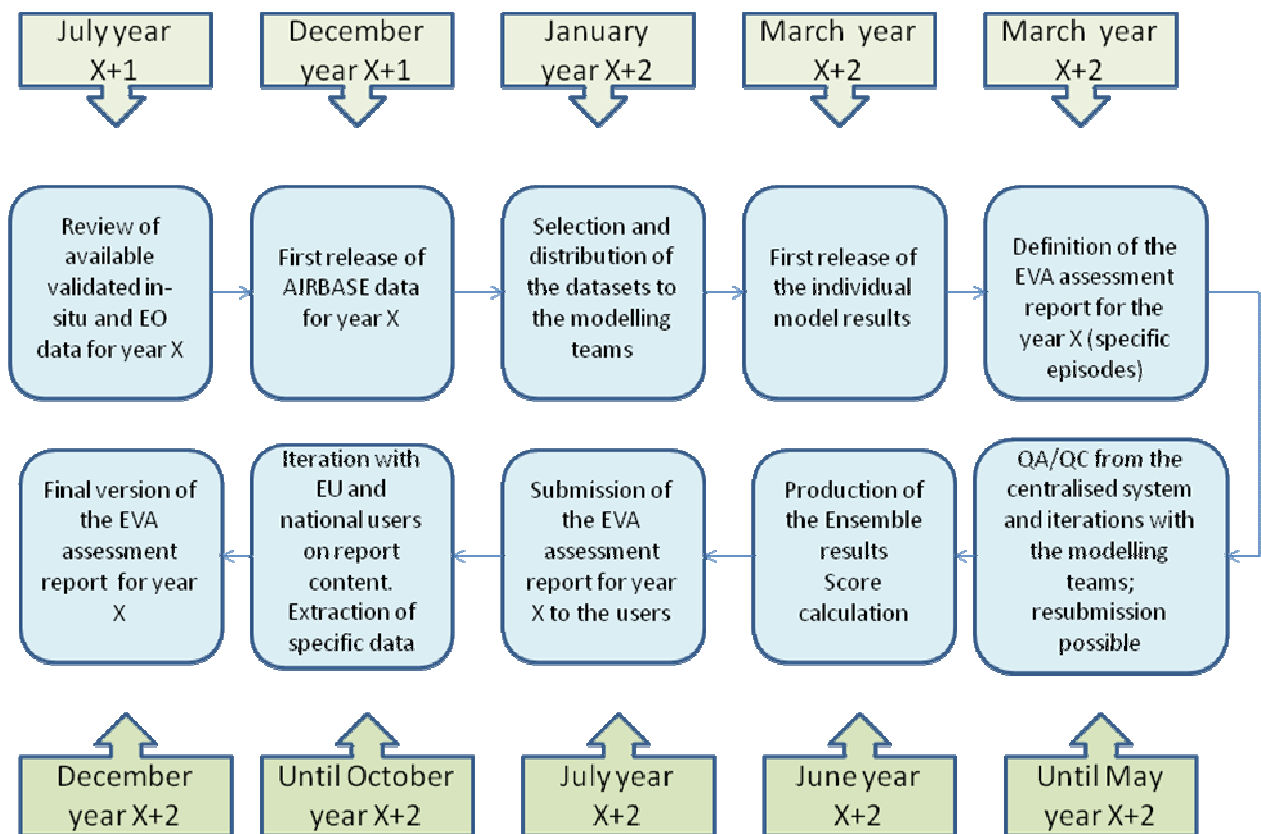


Figure 4. Chronogram presenting the production cycle of the EVA assessment reports

## 2 Status of the individual regional air quality modelling systems

In this paragraph we briefly review the status of the individual modelling chains that were run in MACC for the 2007-2008 and 2009 assessment reports (Table 1) and provide information about what is expected to run in MACC2 (Table 2). This synthesis will provide guidance and specifications to follow the model developments foreseen to deal with the EVA objectives.

Model	Data assimilation chain description	Pollutants assimilated	Observation data assimilated or tested in MACC
CHIMERE	Kriging and Optimal Interpolation approach to correct ground level concentrations Ensemble Kalman filter chain developed in MACC, operational by the end of the project in EDA	Ozone, PM10, NO2	- Only in-situ data from AIRBASE
EMEP	No operational data assimilation chain	-	-
EURAD-IM	Intermittent 3DVAR	O <sub>3</sub> , NO <sub>2</sub> , NO, CO, SO <sub>2</sub> , PM2.5, PM <sub>10</sub>	AIRBASE in situ measurements MOSAIC air borne in situ measurements NO <sub>2</sub> tropospheric column retrievals from OMI, GOME-2, SCIAMACHY MOPITT CO profiles  PM10 SYNAER retrievals : Algorithms available but not yet operationally in use.
LOTOS-EUROS	Ensemble Kalman filter	O <sub>3</sub> , NO <sub>2</sub> , PM <sub>10</sub> , AOD, SO <sub>2</sub> , SO <sub>4</sub>	AIRBASE in-situ data for O <sub>3</sub> and PM <sub>10</sub> OMI for NO <sub>2</sub> , evaluation studies
MATCH	3DVAR with transform into spectral space	O <sub>3</sub> , NO <sub>2</sub> , SO <sub>2</sub> , CO, PM2.5, PM <sub>10</sub> and possibly AOD	AIRBASE in-situ data  Satellite information : retrieval ongoing from OMI, AIRS, MODIS, but not used operationally

MOCAGE	3Dvar operational chain	O3 No additional pollutants included for 2008 and 2009 re-analyses. Work is progressing for operational implementation for NO2, SO2, CO, PM. A paper is in an advanced stage regarding ozone analyses and formulation of time-dependent B (Jaumouillé et al., 2012).	AIRBASE in-situ data  Satellite NO <sub>2</sub> (OMI) and CO (IASI from ULB/LATMOS or EUMETSAT ; MOPITT from NCAR)
SILAM	3Dvar operational chain Operational 4Dvar chain – postponed to MACC-II	O <sub>3</sub> , NO <sub>2</sub> , SO <sub>2</sub>  Extension to PM - not yet done	AIRBASE in situ data

*Table 1. Specification of the data assimilation chains run in MACC for the 2007, 2008, and 2009 assessment reports*

Model	New DA chain	New pollutants	New observation data
CHIMERE	Continuation with OI and implementation of the EnKF chain	CO	OMI and IASI for NO <sub>2</sub> and O <sub>3</sub> and MOPITT for CO
EMEP	Update of the current 3Dvar chain; 4Dvar?	O3 and CO (may be)	IASI O3 column; MOPITT column or profile (maybe)
EURAD-IM	Backup of the assimilation system at Jülich 4Dvar inversion for emissions (not operationally) Account for special events (wild fire, volcanoes, dust outbreaks)	Volcanic Ash, dust	IASI tropospheric ozone profile AOD from SEVIRI, MODIS SYNAER PM10 retrievals
LOTOS-EUROS	Multi-component assimilation with same assimilation code	Same as the MACC chain	Same as the MACC1 chain IASI O3; MOPITT/IASI O3 and CO; PM2.5; satellite AOD (MODIS)
MATCH	EnKF assimilation system could replace in a late phase the current 3DVar system	Chemical composition of PM	SCIAMACHY, OMI, GOME-2, CALIPSO, (IASI), and MODIS
MOCAGE	No, improvement of the current chain	In-situ NO <sub>2</sub> , SO <sub>2</sub> , CO, PM (in addition to ozone).	IASI O <sub>3</sub> and CO columns. Later, NO <sub>2</sub> columns from OMI.

SILAM	4Dvar for a subset of species, improved covariance model for the 3DVar chain	PM, Desert dust and other aerosols, pollens (+ improvement of the model chemical schemes)	OMI tropospheric NO <sub>2</sub> products, SEVIRI and MODIS will be considered for aerosols MOZAIC profiles for the reanalysis product Integration of emission information (dust outbreak, wild fires) through concentration related observations
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*Table 2. Specification of the data assimilation chains to be run for EVA within MACC2*