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MOCAGE

Products, Quality and Background Information

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SEVENTH FRAMEWORK PROGRAMME

MOCAGE facts sheet

1. Products portfolio

Name	Description	Freq.	Available	Species	Time span
FRC	Forecast at the surface, 500m, 1000m, 3000m, and 5000m above ground	Daily	5 UTC	O_3, NO, NO_2, CO, SO_2	0-72h, hourly
ANA	Analysis at the surface, 500m, 1000m, 3000m, and 5000m above ground	Daily	16 UTC	O_3 (other species are modified through assimilation of ozone, but no data assimilated)	0-24h of the day before, hourly

2. Performance statistics

See annexes.

3. Availability statistics

Quarter 10 (September, October, November 2011) : 93% of the MOCAGE forecasts and 100% of analyses have been provided in time.

MOCAGE forecasts were missing for 20 September, 9, 10 October and 19, 21 and 28 November. These delayed forecasts were related to issues downloading IFS meteorological forecasts from ECMWF (line saturated by other applications, specially of operational nature).

4. Assimilation and forecast system: synthesis of main characteristics

Assimilation and Forecast System	
Horizontal resolution	0.2° regular lat-lon grid
Vertical resolution	47 layers up to 0.1 hPa Lowest layer thickness about 40 m About 8 layers below 2 km
Gas phase chemistry	RACM (trospheric) and REPROBUS (stratospheric)
Heterogeneous chemistry	Only reactions on Polar Stratospheric Clouds (stratosphere) yet
Aerosol size distribution	Bins
Inorganic aerosols	*Not implemented in current MACC version*

Secondary organic aerosols	*Not implemented in current MACC version*
Aqueous phase chemistry	Aqueous reactions for sulphate production
Dry deposition/sedimentation	Resistance approach (Michou et al., 2004) for gases, (Nho-kim et al., 2005) for aerosol
Mineral dust	Included: see evaluation in (Martet et al., 2009)
Sea Salt	Included: see evaluation in (Martet, PhD thesis, 2008)
Boundary values	MOCAGE global domain (2°) for all the chemical species with optional relaxation towards G-RG values for species : ozone, CO, HCHO, NO, NO_2, HNO_3, PAN, CH_4, ethane, isoprene
Initial values	24h forecast from the day before
Anthropogenic emissions	TNO (2000) inventory binned at 0.2° resolution, complemented by EMEP 0.5°x0.5° shipping emissions
Biogenic emissions	Fixed monthly biogenic emission, based upon Simpson approach.
Forecast System	
Meteorological driver	12:00 UTC operational IFS forecast for the day before
Assimilation System	
Assimilation method	3d-var
Observations	Ozone in situ data from D-INSITU (other compounds not yet in pre-operational analyses), atmospheric NO_2 columns from AURA/OMI (not yet in the pre-operational analyses)
Frequency of assimilation	Every hour over the day before
Meteorological driver	00:00 UTC operational IFS forecast for the day before

Evolutions in the MOCAGE suite

2011/08/05: new MOCAGE software release (phasing with operational version for Prev'Air, including several bugfixes; aerosol are now activated in order to allow output of PM2.5 and PM10)
2010/12/30: bugfix (scavenging of aerosol in upper atmosphere); though, this was most probably not affecting significantly the version of MOCAGE run for MACC
2010/05/05: new MOCAGE software release (v6: this version includes aerosols but this option was not activated for MACC applications; refined treatment of nitrogen oxides)
2009/12/01: consolidation of IFS meteorological forecast provision (as this was the main cause of delays)
2009/06/01: start of MACC pre-operational forecasts

MOCAGE background information

1. Forward model

The MOCAGE 3D multi-scale Chemistry and Transport Model has been designed for both research and operational applications in the field of environmental modelling. Since 2000, MOCAGE allows to cover a wide range of topical issues ranging from chemical weather forecasting, tracking and backtracking of accidental point source releases, trans-boundary pollution assessment, assimilation of remote sensing measurements of atmospheric composition, to studies of the impact of anthropogenic emissions of pollutants on climate change, with over 40 references in the international refereed literature. For this, MOCAGE offers a flexible structure that allows to adapt the model CPU/MEM requirements and parameterizations to the different applications. MOCAGE has been run daily since 5 years and in 2004, Météo-France joined the partnership consortium and operational platform "Prév'Air" (http://www.prevair.org, Rouil et al., 2009) in charge of the pollution monitoring and forecasting over France.

1.1 Model geometry

MOCAGE considers simultaneously the troposphere and stratosphere at the planetary scale and over limited-area sub-domains at higher horizontal resolution, the model providing (by default) its own time-dependent chemical boundary conditions. For MACC, MOCAGE configuration comprises a global domain (2°) and the MACC regional domain (0.5°, 15°W-35°E and 35°N-70°N). Only the products on the MACC domain are used for the regional services. In the vertical, 47 hybrid (σ,P) levels go from the surface up to 5 hPa, with approximately 8 levels in the Planetary Boundary Layer (ie below 2km), 16 in the free troposphere and 24 in the stratosphere. The thickness of the lowest layer is about 40 m.

1.2 Forcing and boundary values

Depending upon applications, MOCAGE can run in both on-line, coupled to a general circulation model for climate studies for instance, or off-line modes, forced by archived meteorological analyses or forecasts. The off-line configuration can use Météo-France ARPEGE, ALADIN and AROME or ECMWF/IFS operational Numerical Weather Prediction products. In MACC, the IFS daily operational forecast are used: 0-84h three hourly forecasts of horizontal winds, humidity and surface pressure are taken from the 1200 suite.

The values over the global MOCAGE domain are constrained (relaxation) by the three-hourly G-RG values for available species: ozone, CO, HCHO, NO, NO_2, HNO_3, PAN, CH_4, ethane, isoprene. The use of MOCAGE global domain help introducing smoothly, on the horizontal as well as on the vertical, these chemical boundary conditions into the regional MACC domain.

Chemical initial values are provided by MOCAGE 24h forecast from the day before. Though data assimilation is available (see hereafter), it is not currently activated in the MACC forecast suite.

1.3 Dynamical core

The dynamical forcings from IFS (hydrostatic winds, temperature, humidity and pressure) feed the advection scheme, as well as the physical and chemical parameterizations. Forcings are read-in every 3 hours, and are linearly interpolated to yield hourly values, which is the time-step for advection; smaller time-steps are used for physical processes and chemistry, but the meteorological variables are kept constant over each hour. MOCAGE is based upon a semi-lagrangian advection scheme (Williamson and Rasch, 1989), using a cubic polynomial interpolation in all three directions. Evaluation of transport in MOCAGE using Radon-222 experiments can be found in (Josse et al., 2004).

1.4 Physical and chemical parameterizations

Concerning physical and chemical parameterizations, an operator splitting approach is used. Parameterizations are called alternatively in forward and reverse order, with the objective to reduce systematic errors. Several options are available within MOCAGE; we briefly mention here the options used for MACC.

1.4.1 Photolysis frequencies

Photolyses are taken into account using a multy-entry look-up table computed off-line with the TUV software version 4.6 (Madronich, 1987). Photolyses depend on month (including monthly aerosol climatologies), solar zenith angle, ozone column above each cell (as the model extends to the mid-stratosphere, it is actually the ozone profile computed by MOCAGE which is used at every timestep), altitude and surface albedo in the UV. They are computed for clear-sky conditions and the impact of cloudiness on photolysis rates is applied afterwards.

1.4.2 Aerosol module

The aerosol module of MOCAGE is now activated. The species currently included are: dusts, black carbon, sulphate, sea salts, as well as primary PM2.5 and PM10. Thus, currently not all aerosol species (other inorganic, secondary organic aerosol) are accounted for in this version. A low bias is expected for PM10 and PM2.5. Details on MOCAGE aerosol simulation evaluation can be found in (Martet et al., 2009; Martet, PhD, 2008) for dusts, (Nho-Kim et al., 2005) for black carbon and (Ménegoz et al., 2009) for sulphate. The representation of other aerosol species is an on-going development at MF-CNRM.

1.4 Dry deposition and sedimentation

A description of MOCAGE surface exchanges module is presented in (Michou and Peuch, 2002), as well as in (Michou et al., 2004). The dry deposition parameterization relies on a fairly classical surface resistance approach (Wesely, 1989), but with a refined treatment of the stomatal resistance, similar to the one used in Météo-France NWP models: see description of the ISBA original approach in (Noilhan and Planton, 1989).

Sedimentation of aerosol follows (Nho-Kim et al., 2004).

1.4.3 subgrid convective clouds

For sub-gridscale transport processes, vertical diffusion is treated following (Louis, 1979) and transport by convection is from (Bechtold et al., 2001). Scavenging within convective clouds is following (Mari et al., 2000), allowing to compute wet removal processes directly within the convective transport parameterisation. Wet deposition in stratisform clouds and below clouds follows (Giorgi and Chameides, 1986).

1.5 Chemistry

1.5.1 Gas phase

MOCAGE configuration for MACC comprises 118 species and over 300 reactions and photolyses. It is a merge of reactions of the RACM scheme (Stockwell et al., 1997) with the reactions relevant to the stratospheric chemistry of REPROBUS (Lefèvre et al., 1994). Evaluation at the intercontinental scale can be found in (Bousserez et al., 2008) ; evaluation for air quality applications are discussed in (Dufour et al., 2004).

1.5.2 Aqueous phase

Aqueous chemistry for the formation of sulphate is represented. See (Ménegoz et al., 2009) for details.

1.5.3 Aerosol phase

Detailed heterogeneous chemistry on Polar Stratospheric Clouds (types I, II) is accounted for, as described in (Lefèvre et al., 1994).

Other heterogeneous chemistry processes are currently not included.

2. Assimilation system

Any assimilation algorithm can be seen as a sequence of elementary operations or elementary components that can exchange data (Lagarde et al., 2001). Based on this idea, CERFACS has developed a coupling software PALM software (www.cerfacs.fr/~palm), that manages the dynamic launching of the components of assimilation systems (forecast model, algebra operators, I/O of observational data,...) and the parallel data exchanges.

MACC operations will use the assimilation system based upon MOCAGE and PALM, which has been developed and evaluated during the ASSET European project (Geer et al., 2006; Lahoz et al., 2007). This system is particularly versatile, as both the CTM degree of sophistication (for instance, the number of chemical tracers involved, the physical or chemical parameterisations, the horizontal and vertical geometries,…) and the data assimilation technique used via PALM can be changed easily. Current available options are 3D-VAR, 3D-FGAT and incremental 4D-VAR methods to assimilate profile and column data for key measured atmospheric constituents, by means of a generic observation operator component. As a first approximation, background error standard deviations are prescribed as proportional to background amounts. In order to spread assimilation increments spatially, background error correlations are modelled using a generalized diffusion operator (Weaver and Courtier 2001). Several data assimilation experiments have been published with MOCAGE, both for the stratosphere and troposphere (see for instance Pradier et al., 2006 or El Amraoui et al., 2008).

In MACC, a 3D-VAR technique has been implemented. The first version of the MOCAGE assimilation suite (from July 1st 2010 on and for R-EVA re-analyses for 2008 and 2009) considers only surface ozone. The assimilation window is 1h every hour.

3. Development plan

The next development steps for the MACC MOCAGE version are, beyond routine integration of new model developments at Météo-France:

- extension of aerosol species represented in MOCAGE
- introduction of fire emissions based upon the MSG/SEVIRI FRP algorithm (output of D-FIRE workpackage)
- extension of surface *in-situ* (CO, SO_2, NO_2) assimilated in the pre-operational data assimilation

4. References

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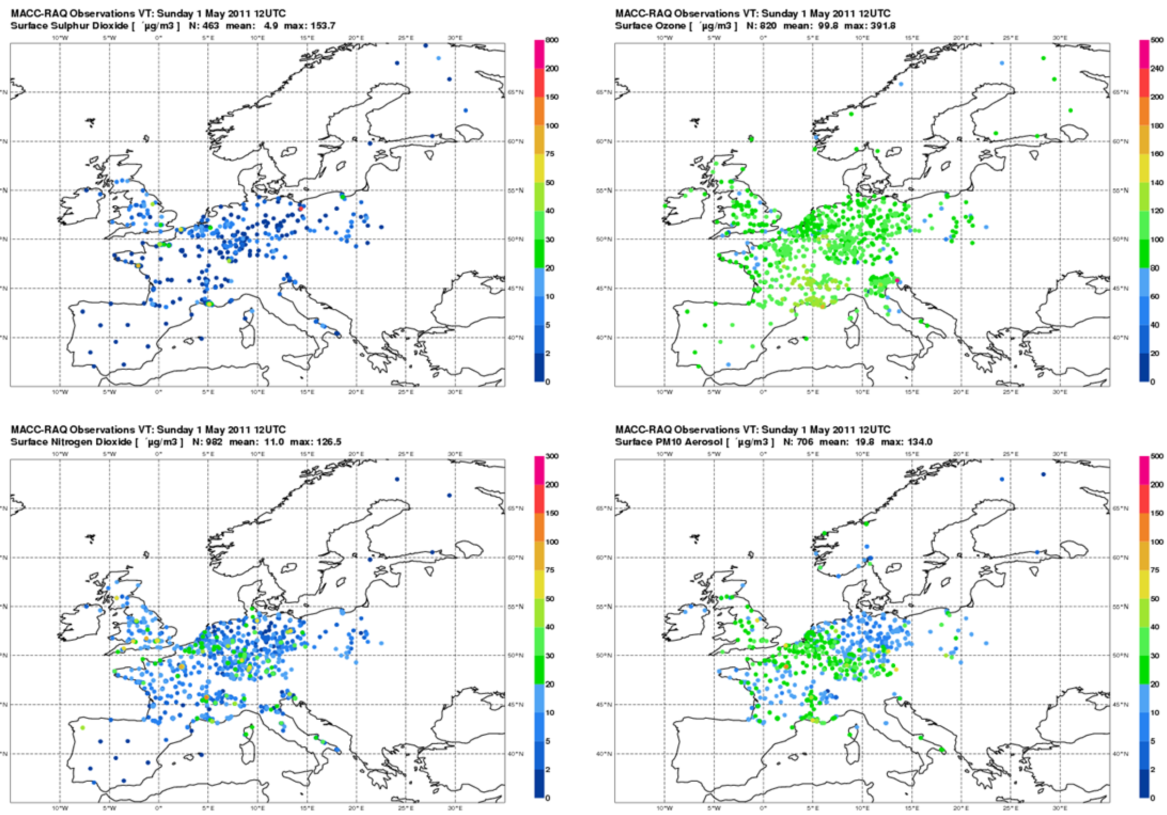
Verification report for quarter #10

This verification report covers the period September/October/November 2011. For this report, average skill scores (bias, root mean square error, correlation) for the MOCAGE model are successively presented for two pollutants : ozone and NO_2. The skill is shown for the entire forecast horizon 0 to 72h (3-hourly values), allowing to evaluate the entire diurnal cycle and the evolution of performance from day 1 to day 3.

For this verification period, as was the case on the MACC website, verifications are performed against all available data in Near-Real-Time (NRT) for the following countries: Belgium, Czech Republic, Denmark, Finland, France, Germany, Greece (Athens area only), Italy (not all regions), Netherlands, Norway, Poland, Spain, Sweden and the United Kingdom. The total number of sites is typically up to: 900 for ozone, 1200 for NO_2, 550 for SO_2, 300 for CO, 900 for PM10. As an example, the data coverage for Sunday May 1st 2011 12UTC is depicted below.

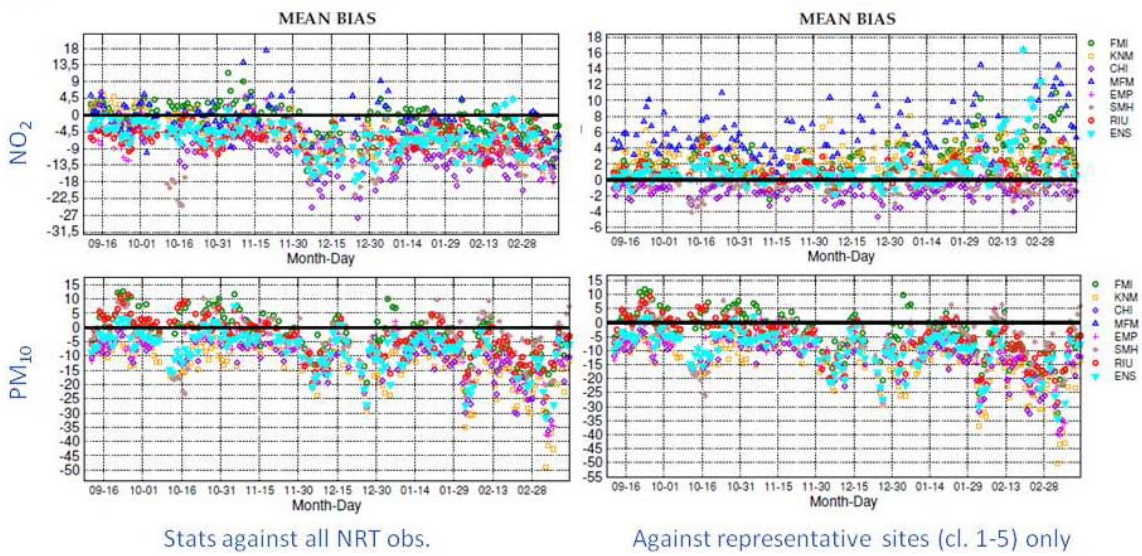


Near-Real-Time data coverage (May 1st 2011, 12 UTC)

Within MACC, the D-INSITU subproject is working with the European Environment Agency (EEA) to set up a new, more extensive and robust Near-Real-Time dataflow. An EEA European Air Quality data stream is available since the spring of 2011 and it has been checked by D-INSITU partners (in particular NILU) against the data currently received by

MACC in NRT, which results from *ad hoc* bilateral agreement with Environment Agencies in 14 different countries. While there is an overlap between the two datasets, there is still a considerable number of differences. Briefly, the EEA dataset has more reporting sites for ozone and less for the other species. Also, there is a great interest in attempting to merge the two data sources, by helping for instance EEA to get access to data in the countries with which GEMS-MACC has been in contact and which do not provide all their NRT data to EEA. While this does not change the general objective to move to a EEA-based dataflow, it was felt that this evolution was not yet readily feasible for the last periods of MACC; this will accomplished in MACC-II. A further advantage will be that data will arrive sooner, typically less than 3 hours after measurement. Currently, hourly data from the day before are available to MACC between 2 and 10 UT every day, depending on the country: this delays the possible start of daily verification calculations and makes it impossible to base the daily forecasts upon the analysis of the day before -as forecasts have to be delivered early enough every morning, in order to serve users' needs.

For the NRT verification of forecasts, the typology of sites is currently not taken into account: there is no uniform and reliable metadata currently for all regions and countries, which have all different approaches to this documentation. Skill scores are thus computed using all the data received. Within MACC, work has been carried out [Joly and Peuch, 2012] to build an objective classification of sites, based on the past measurements available in Airbase (EEA) ; see D_R-ENS_5.1 for more details. This classification can now be used in order to restrict verification only to the sites that have a sufficient spatial representativeness. Currently, about half of the sites used in the verification are declared "urban" in Airbase metadata and would be in principle not representative enough for comparing against forecast models that have horizontal resolutions of approximately 0.2°. However, our findings indicate that a significant fraction of sites labelled "urban" or "suburban" has actually little local character (as seen in past time series of measurements) and could be in fact more representative than what could be inferred from the metadata information. The figure below shows scores computed using all MACC data available in NRT and using only data for sites from classes 1-5 of our objective classification (the "background" fraction).



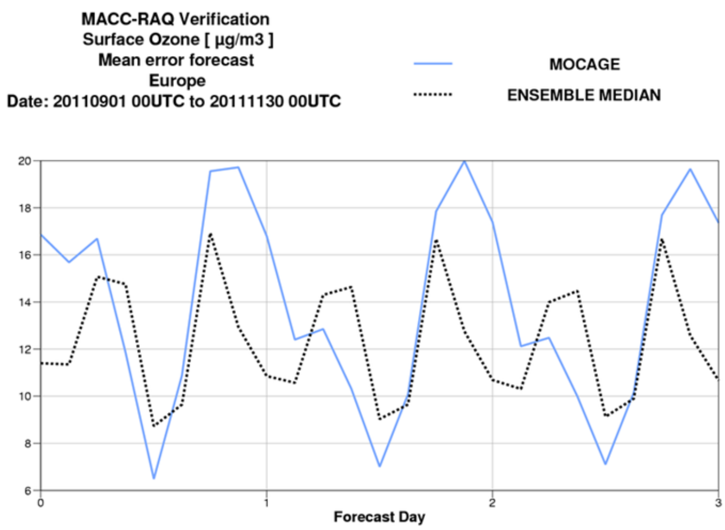
Sample model verification for the period 15/09/2010 to 28/02/2011 using all NRT sites (left) and using only most representative sites (classes 1-5) only (right). Values are for NO_2 (top) and PM10 (bottom) for 0300 UTC.

While the statistical approach using only representative sites -according to the objective classification- is clearly the way forward (as it does not also thin too much the NRT data available), we see that overall skill scores are in general not too much affected by the observations from sites that have a local character, as illustrated here for PM10. Noticeable exceptions are winter night-time NO_2 values (top row on the figure), for which the general negative bias of the ensemble (around 5 $\mu g.m^{-3}$) and of most of the individual models is entirely offset by using representative data only to compute skill scores.

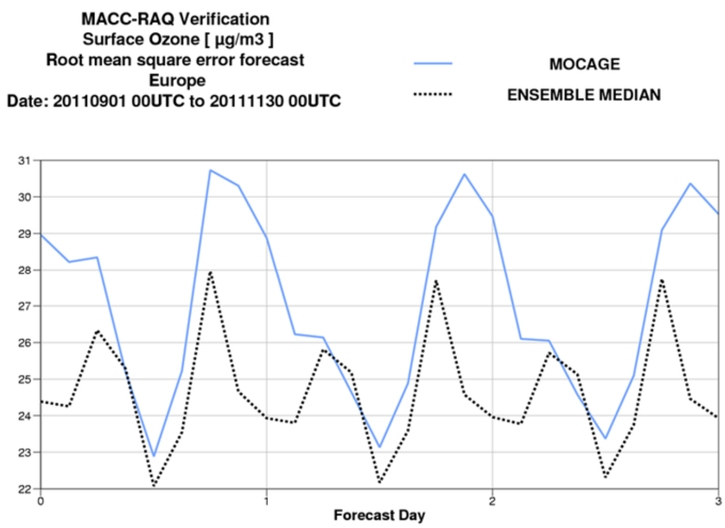
As this evolution does not induce dramatic changes to our assessment, we have opted to finalise MACC using “all NRT data” statistics (to have continuity of approach during the project) and to switch to the “representative sites only” statistics only from the first quarter of MACC-II (DJF 2011-2012). This approach will also contribute to alleviate the issue of the large variation in site densities from one country to another: the countries with higher densities of observational sites, particularly Germany and France, will actually “loose” many more sites than the others (also in proportion). Yet, the issue remains that the overall skill scores presented here, and also on the MACC website in NRT, are largely governed by the behaviour of the models in the “data intensive” countries. In MACC-II, our verification procedures will be more segmented (by countries and by large continental regions: Northern Europe, Eastern Europe, Mediterranean...), which will allow to be increasingly more specific on the description of AQ products quality. At the same time, we acknowledge that the amount of information provided has to remain within reasonable bounds, in order not to confuse general users.

Joly, M. and V.-H. Peuch, 2012: Objective Classification of air quality monitoring sites over Europe, Atmos. Env., ***47****, 111-123.*

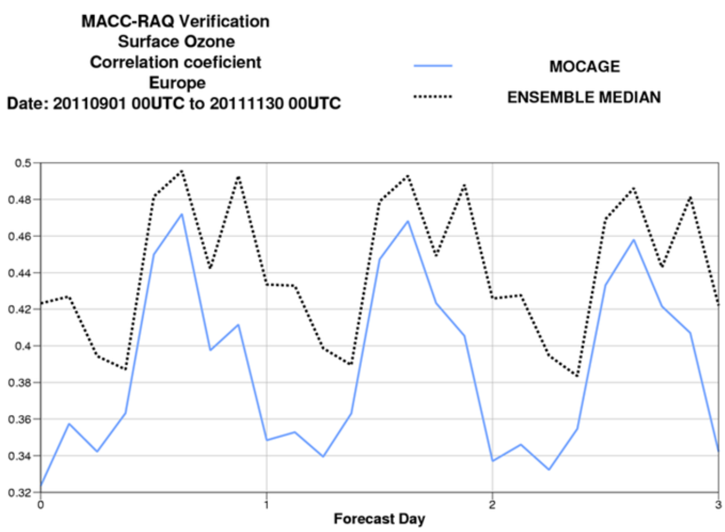
MOCAGE: ozone skill scores, period #10 (September, October, November 2011)



For this period, MOCAGE and the ENSEMBLE median are comparable in terms of bias: MOCAGE is better in the morning and till mid-afternoon, while ENSEMBLE is better in the end of afternoon and night. Compared to the same period of the year in 2009 and 2010, both MOCAGE and the ENSEMBLE have improved noticeably.

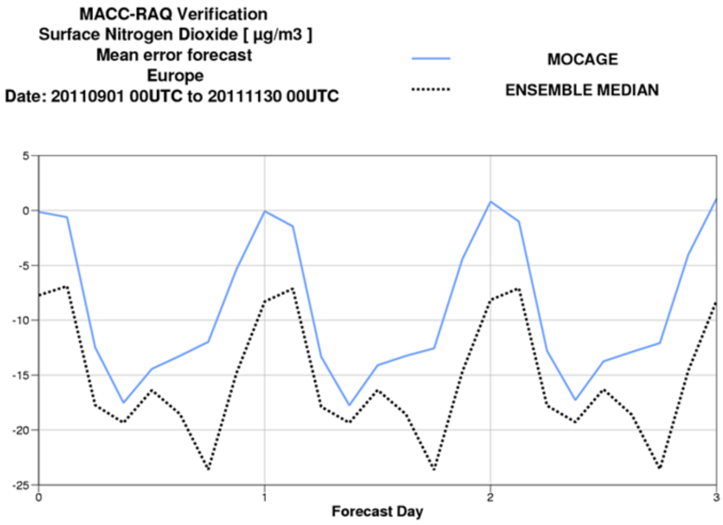


The RMSE is better for ENSEMBLE than for MOCAGE, particularly at night. They are equivalent in the morning period.

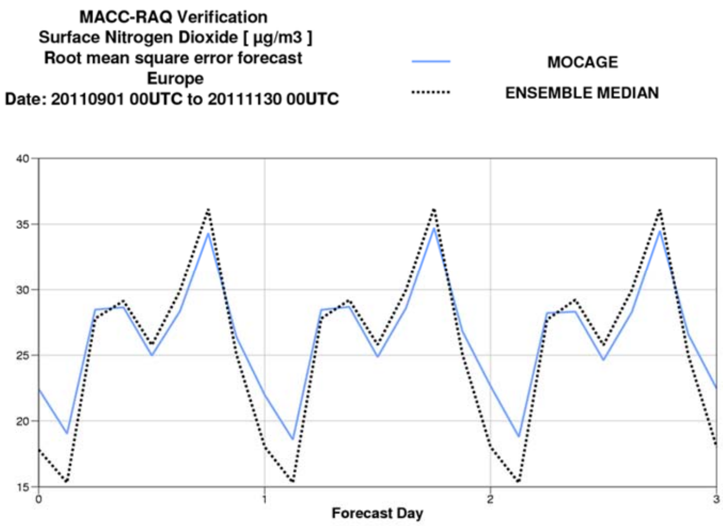


ENSEMBLE is superior to MOCAGE in terms of correlation throughout the day. ENSEMBLE has significantly improved (more than MOCAGE) compared to 2009 and 2010, reaching almost 0.5.

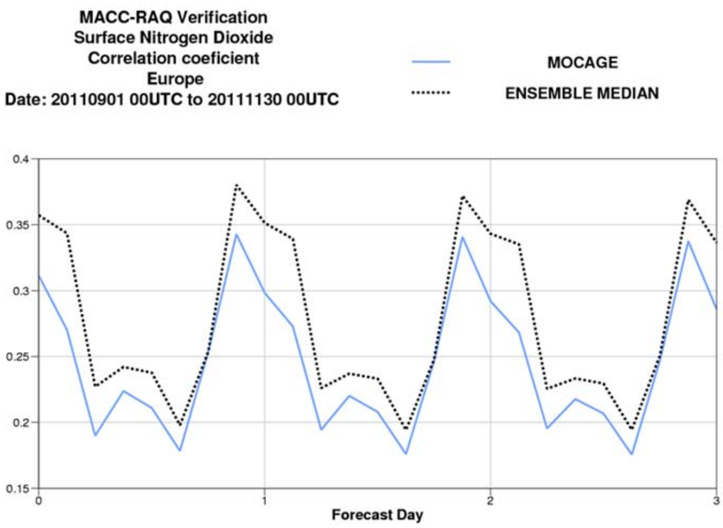
MOCAGE: NO_2 skill scores, period #10 (September, October, November 2011)



As it is generally the case for NO_2, MOCAGE is better than the ENSEMBLE median in terms of bias, with (again) almost no bias around midnight.



MOCAGE and the ENSEMBLE median are equivalent in terms of RMSE. This is a clear progress for MOCAGE compared to past periods. The change of code in early August is probably responsible for this improvement.



The correlations behave similarly for MOCAGE and the ENSEMBLE median, remaining however both relatively low. For this period and this parameter (autumn, NO_2), there is certainly an impact from the fact that the site types are not filtered: the scores are influenced by some sites with a urban/local character, that the models (at the current horizontal resolution) cannot reproduce.