

MOCAGE Fact sheet

1.1 Assimilation and forecast system: synthesis of the main characteristics

Discretisation	Horizontal resolution	0.1° x 0.1° regular lat-lon
	Number of vertical levels	47
	Top altitude	5hPa
	Depth of lower most layer	40m
	Number of lower layers	8 below 2km
Initial & boundary conditions & meteorology	Meteorological driver	D-1 12:00 UTC IFS for FC, 1hrly (from +00h to +72h), 3hrly (from +72h to +96h) ; D00:00 UTC IFS for AN, 1hrly
	Boundary values	CAMS-Global IFS + MOCAGE global for additional species
	Initial values	Previous forecast
Emissions: natural & biogenic	In-domain soil and road dust emissions	Sic et al., 2014
	In-domain sea-salt emissions	Sic et al., 2014
	Birch, Grass, Olive, Ragweed, Alder, Mugwort Pollen provided by FMI	yes
	Biogenic emissions	MEGAN-MACC climatology isoprene from MEGAN v2.04 (Gunther et. al 2006)
	Soil NOx	GEIA Yienger, J. J., and Levy, H. (1995), Empirical model of global soil-biogenic NO _x emissions, J. Geophys. Res., 100(D6), 11447– 11464, doi:10.1029/95JD00370.
	Wildfires emissions	Hourly emissions from D-2 cycled for AN (D-1) and FC (D+0 and D+1, zero for the remaining days)
Chemistry/ Physics	Gas phase chemistry	RACM (tropospheric) and REPROBUS (stratospheric)
	Heterogeneous chemistry	only relevant for polar stratospheric clouds
	Aerosol size distribution	6 bins
	Inorganic aerosols	ISORROPIA-2 (Guth et al., 2016)
	Secondary organic aerosols	not included
	Aqueous phase chemistry	SO ₂ oxidation
	Dry deposition: gases	resistance approach (Michou et al., 2004)
	Dry deposition: aerosols	Sič et al., (2015)
	Wet deposition	Convective: Mari et al, 2000 Stratiform: Giorgi and Chameides (1986), Slinn (1977), Slinn (1982)
Assimilation	Assimilation method	3D VAR
	Assimilated surface pollutants	NO ₂ , O ₃ , PM _{2.5} , PM ₁₀
	assimilated satellite	ground-based lidars from French network
	Frequency of assimilation	Hourly

1.2 Model Overview

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 has been allowing 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.

1.3 Model geometry

For the CAMS Regional Service, MOCAGE operates on a regular latitude-longitude grid at 0.1 resolution for both forecast and assimilation. The products delivered for the CAMS service are issued from the regional domain only. In the vertical, 47 hybrid levels go from the surface up to 5 hPa, with approximately 8 levels in the Planetary Boundary Layer (i.e. below 2km), 16 in the free troposphere and 24 in the stratosphere. The thickness of the lowest layer is about 40 m. There is no downscaling applied to surface concentration.

1.4 Forcing Meteorology

The forcing meteorology is retrieved from the IFS model vertical layers covering the MOCAGE vertical extent on a $0.1^\circ \times 0.1^\circ$ horizontal grid resolution with a temporal resolution of one hour for the 3 first forecast days and 3 hours for the last forecast day. The forecast released at 12UTC of the previous days is used. The meteorological parameters used are : horizontal winds, humidity and surface pressure.

1.5 Chemical initial and boundary conditions

Chemical initial values in the regional domain are provided by MOCAGE 24h forecast from the day before.

The boundary conditions are taken from global CAMS operational suite for the species (chemical and aerosols) that are distributed (see Table 2). For aerosols, the 2 or 3 bins from IFS are summed to get total concentration and then distributed onto the 6 MOCAGE bins considering Mean IFS bin size as emission modes. A factor 4.3 is applied to convert Sea Salt from wet to dry fractions. Aerm03 (of diameter larger than $10\mu\text{m}$) is only marginally distributed within MOCAGE PM10 sea salt because of the matching between bins and log-normal modes. For the species not included in Table 2, the concentrations from the MOCAGE global domain are used, which helps to introduce smoothly, on the horizontal as well as on the vertical, these chemical boundary conditions into the CAMS regional domain.

1.6 Emissions

The common annual anthropogenic emissions CAMS-REG are implemented as explained in Section 3.2. Temporal disaggregation is based on the GENEMIS tables (Ebel et al., 1997), using a GNFR to SNAP matrix.

Concerning biomass burning sources, GFAS emissions are emitted according an 'umbrella' profile, with a maximum injecting height climatologically determined. GFAS "near real time" observation-based fire emissions are made available with a 8-hr delay. So that when the forecast system is initiated, most GFAS emission cover Day-2 of the forecast to be produced. As a consequence, the 2-day persistence is interpreted in a way that fire emissions are only applied for D+0.

1.7 Solver, advection and mixing

Concerning physical and chemical parameterisations, an operator splitting approach is used. Parameterisations are called alternatively in forward and reverse order, with the objective to reduce systematic errors.

Meteorological forcings are read every 3 hours from IFS input data, 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 3 directions.

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 stratiform clouds and below clouds follows Giorgi and Chameides (1986).

1.8 Deposition

A description of MOCAGE surface exchanges module is presented in Michou et al. (2004). The dry deposition parameterisation 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 Meteo-France numerical weather prediction models (Noilhan and Planton, 1989). Sedimentation of aerosol follows (Nho-Kim et al., 2004).

1.9 Chemistry and aerosols

The MOCAGE configuration for CAMS comprises 118 species and over 300 reactions and photolysis. 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). Aqueous chemistry for the formation of sulphate is represented, following (Ménégoz et al., 2009). 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.

Photolysis is taken into account using a multi-entry look-up table computed off-line with the TUV software version 4.6 (Madronich, 1987). Photolysis depends 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 time step), 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.

The aerosol module of MOCAGE includes the primary species dusts, black carbon, sea salts, organic carbon, and the secondary inorganic species sulphate, nitrate and ammonium. The

formation and the multi-phasic equilibrium of inorganic secondary aerosols are modelled by the ISORROPIA-II module. Details on MOCAGE aerosol simulation evaluation can be found in Martet et al. (2009) for dusts, in Nho-Kim et al. (2005) for black carbon, and in Sic et al. (2015) for the latest version of MOCAGE primary aerosol module. The implementation and the evaluation of secondary inorganic aerosols in MOCAGE are described by Guth et al (2016). Further improvements of the representation of aerosols in MOCAGE are expected in the future with on-going work regarding organic secondary aerosols.

1.10 Assimilation system

MOCAGE operations for CAMS use the assimilation system based upon MOCAGE and PALM (Lahoz et al., 2007). 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 assimilation strategies are available in PALM but for CAMS MOCAGE uses a 3D-VAR technique, with an assimilation window that is 1h every hour. MOCAGE assimilates O₃, NO₂, PM₁₀ and PM_{2.5} in-situ surface observations. The species are assimilated independently every hour without any cross-species covariances, and then the increments per species are added to the analysis that serves as initial condition for computing the background of the next hour of the assimilation process.