7. MOCAGE factsheet

7.1 Assimilation and forecast system: synthesis of the main characteristics

Assimilation and forecast system	
Horizontal resolution	0.1° regular lat-lon grid for forecast 0.1° regular lat-lon grid for assimilation
Vertical resolution	47 layers up to 5 hPa Lowest layer thickness about 40 m About 8 layers below 2 km
Gas phase chemistry	RACM (tropospheric) and REPROBUS (stratospheric)
Heterogeneous chemistry	Only reactions on Polar Stratospheric Clouds (stratosphere) yet
Aerosol size distribution	Bins
Inorganic aerosols	Included: ISORROPIA module (Guth et al, 2016)
Secondary organic aerosols	Not implemented in current CAMS 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 by Sic et al. (2014)
Sea Salt	Included: see evaluation by Sic et al. (2014)
Boundary values	Values delivered by global CAMS and MOCAGE global domain (2°) for the other chemical species
Initial values	24h forecast from the day before
Anthropogenic emissions	CAMS-REG-AP_v3.1/2016 (before Nov 2020) CAMS-REG-AP_v4.2/2017 (after Nov 2020)
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	O3, NO2 and PM10/PM2,5 in-situ data distributed by Meteo-France
Frequency of assimilation	Hourly
Meteorological driver	00:00 UTC operational IFS forecast

7.2 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 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, with over 60 references in the international refereed literature. For this, the MOCAGE structure offers flexibility to tailor the model CPU/MEM requirements and parameterisations to the different applications. MOCAGE has been running daily since 2005. Meteo-France joined in 2004 the partnership consortium and operational platform 'PREV'AIR' (Rouil et al., 2009), in charge of the pollution monitoring and forecasting over France.

7.2.1 Model geometry

MOCAGE simultaneously considers 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 the CAMS Regional production, the MOCAGE configuration comprises a global domain (2° resolution) and the regional domain (25°W-45°E and 30°N-70°N 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 (σ, P) 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.

7.2.2 Forcings and boundary conditions

7.2.2.1 Meteorology

The MOCAGE configuration that has been developed and operated since the MACC project runs in off-line mode, forced by IFS meteorological analyses or forecasts. For the daily forecast production, the IFS daily operational forecasts are used: 0-108h (to cover the 96h forecast time range) 3 hourly forecasts of horizontal winds, humidity and surface pressure are taken from the 12 UTC suite. For the daily analysis production, the same fields are taken from the 00 UTC IFS suite.

7.2.2.2 Chemistry

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 1). For aerosols, the 2 or 3 bins from C-IFS are summed to get total concentration and then distributed onto the 6 MOCAGE bins considering Mean C-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 10µm) is only marginally distributed within MOCAGE PM_{10} sea salt because of the matching between bins and log-normal modes. For the other species, 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.

Table 7. The chemical and aerosol species taken from C-IFS and used in MOCAGE

C-IFS Species	Coupled to MOCAGE Species
go3	O_3
CO	CO
SO_2	SO_2
aermr01, aermr02, aermr03	Sea salt (6 bins)
aermr04, aermr05, aermr06	Desert dust (6 bins)
aermr07, aermr08	Organic carbon (6 bins)
aermr09, aermr10	Black carbon (6 bins)

7.2.2.3 Surface emissions

Surface emissions are pre-processed using the SUMO2 pre-processor. Anthropogenic emissions from CAMS-REG-AP_v3.1/2016 are used until U3 upgrade (Nov. 2020). After, anthropogenic emissions from CAMS-REG-AP_v4.2/2017 are used. Concerning biomass burning sources, GFAS emissions are emitted according an 'umbrella' profile, with a maximum injecting height climatologically determined. A 2-days persistency is applied (i.e. day-2 fires are applied on J0 only).

7.2.3 Dynamical core

The dynamical forcings from IFS (hydrostatic winds, temperature, humidity and pressure) feed the advection scheme, as well as the physical and chemical parameterisations. 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 3 directions. Evaluation of transport in MOCAGE using Radon-222 experiments can be found in (Josse et al., 2004).

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.

7.2.4 Physical parameterisations

Several options are available within MOCAGE; we briefly mention here the options used for the CAMS Regional production.

7.2.4.1 Turbulence and convection

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).

7.2.4.2 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 NWP models: see description of the ISBA original approach in (Noilhan and Planton, 1989). Sedimentation of aerosol follows (Nho-Kim et al., 2004).

7.2.5 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 (Ménegoz 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 sulfate, 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.

7.3 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 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, etc.) and the parallel data exchanges.
MOCAGE operations for CAMS use the assimilation system based upon MOCAGE and PALM, which has been developed and evaluated during the European ASSET project (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, etc.) 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.

Based on past experience, MOCAGE for CAMS uses a 3D-VAR technique, with an assimilation window that is 1h every hour. MOCAGE assimilates O_3, NO_2 and PM_{10} and $PM_{2.5}$ in-situ surface observations for re-analyses and for NRT analyses. 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 at initial condition for computing the background of the next hour of the assimilation process.