2. CHIMERE factsheet

2.1 Assimilation and forecast system: synthesis of the main characteristics

Assimilation and forecast system	
Horizontal resolution	0.1°x0.1°
Vertical resolution	Variable, 9 levels from the surface up to 500 hPa; 7 levels below 2 km
Gas phase chemistry	MELCHIOR2, comprising 44 species and 120 reactions (Derognat, 2003)
Heterogeneous chemistry	NO_2, HNO_3, N_2O_5
Aerosol size distribution	10 bins from 10 nm to 40 µm
Inorganic aerosols	Primary particle material, nitrate, sulphate, ammonium
Secondary organic aerosols	Biogenic, anthropogenic
Aqueous phase chemistry	Sulphate
Dry deposition/sedimentation	Classical resistance approach
Mineral dust	Dusts are considered coming from BC and emitted by desert area inside the domain
Sea Salt	Inert sea salt
Boundary values	Values provided by CAMS global
Initial values	24h forecast from the day before
Anthropogenic emissions	CAMS-REG-AP_v3.1/2016
Biogenic emissions	MEGAN
Forecast system	
Meteorological driver	00:00 UTC operational IFS forecast from the day before
Assimilation system	
Assimilation method	Kriging-based analysis
Observations	Surface ozone, NO_2, PM_{10} and $PM_{2.5}$
Frequency of assimilation	Every hour over the day before
Meteorological driver	00:00 UTC operational IFS forecast for the day before

2.2 Forward model

The CHIMERE multi-scale model is primarily designed to produce daily forecasts of ozone, aerosols and other pollutants, and to make long-term simulations for emission control scenarios. CHIMERE runs over a range of spatial scale from the regional scale (several thousand kilometres) to the urban

scale (100-200 Km), with resolutions from 1-2 Km to 100 Km. The chemical mechanism (MELCHIOR) is adapted from the original EMEP mechanism. Photolytic rates are attenuated using liquid water or relative humidity. Boundary layer turbulence is represented as a diffusion (Troen and Mahrt, 1986, BLM). Vertical wind is diagnosed through a bottom-up mass balance scheme. Dry deposition is as in Wesely (1989). Wet deposition is included. 6 aerosol sizes are represented as bins in the model. Aerosol thermodynamic equilibrium is achieved using the ISORROPIA model. Several aqueous-phase reactions are considered. Secondary organic aerosols formations are considered. Advection is performed by the PPM (Piecewise Parabolic Method) 3d order scheme for slow species. The numerical time solver is the TWOSTEP method. Its use is relatively simple, provided input data is correctly supplied. It can be run with several vertical resolutions, and with a wide range of complexity. It can be run with several chemical mechanisms, simplified or more complete, with or without aerosols.

2.2.1 Model geometry

CHIMERE is a Eulerian deterministic model, using variable resolution in time and space (for Cartesian grids).

The model uses any number of vertical layers, described in hybrid sigma-p coordinates. The model runs over the CAMS domain with a 0.1°x0.1° resolution and 9 vertical levels, extending from the surface up to 500 hPa.

The concentrations provided at the surface is the concentration of the first level of CHIMERE. No vertical downscaling approach is set-up.

2.2.2 Forcings and boundary conditions

2.2.2.1 Meteorology

Within CAMS, CHIMERE is directly forced by the IFS forecasts from the daily operational products delivered at 00 UTC.

2.2.2.2 Chemistry

Boundary conditions can be either "external", or given by a coarse resolution CHIMERE simulation.

The CAMS regional forecasts of CHIMERE use the global CAMS production forcing from C-IFS (see Table 2). In case the production is delayed, a back-up forcing is available with a climatology built on 5 years of the MACC/CAMS re-analysis.

Use of Sea Salt boundary conditions was suspended in the past due to high overestimation. The corrective approach will be implemented before the end of 2019.

Table 2. The chemical and aerosol species taken from C-IFS and used in CHIMERE

C-IFS Species	Coupled to CHIMERE Species
SO_4 (0.06-1.0)	H_2SO_4 (bins 3-4-5-6)
OM (0.06-1.0)	AnBmP BiA1D BiBmP (bins 3-4-5-6)
BC (0.06-1.0)	BCAR (bins 3-4-5-6)
OM (0.06-1.0)	OCAR (bins 3-4-5-6)
DUST1 (0.06-1.1)	DUST (bins 3-4-5-6)
DUST2 (1.1-1.8)	DUST (bin 7)
DUST3 (1.8-40)	DUST (bins 7-8-9-10)
C_2H_6	C_2H_6
CH_2O	HCHO
CH_4	CH_4
CO	CO
HNO_3	HNO_3
ISOP	C_5H_8
NO_2	NO_2
GO_3	O_3
PAN	PAN
SO_2	SO_2

2.2.2.3 Land use

The proposed domain interface is based on the Global Land Cover Facility (GLCF): http://glcf.umiacs.umd.edu/data/landcover 1kmx1km resolution database from the University of Maryland, following the methodology of Hansen et al. (2000, J. Remote Sensing).

2.2.2.4 Surface emissions

The surface emissions are from the TNO emission inventory for anthropogenic emissions. Biogenic emissions are calculated online with the MEGAN module.
Hourly GFAS Fire emissions are downloaded daily from the dedicated Copernicus service through the MARS interface, use of ECPDS is under investigation.
Dust emissions are calculated online within CHIMERE.

2.2.3 Dynamical core

3 advection schemes are implemented: the Parabolic Piecewise Method (PPM, a 3-order horizontal scheme, after Colella and Woodward, 1984), the Godunov scheme (Van Leer, 1979) and the simple upwind first-order scheme.

2.2.4 Physical parameterisations

2.2.4.1 Turbulence and convection

Vertical turbulent mixing takes place only in the boundary layer. The formulation uses K-diffusion following the parameterisation of [Troen and Mahrt, 1986], without counter-gradient term.

2.2.4.2 Deposition

Dry deposition is considered for model gas species i and is parameterised as a downward flux F(d,i)= -v(d,i) c(i) out of the lowest model layer with c(i) being the concentration of species i. As commonly, the deposition velocity is described through a resistance analogy [Wesely, 1989]. The wet deposition follows the scheme proposed by [Loosmore, 2004].

2.2.5 Chemistry and aerosols

In order to decrease the computing time, a reduced mechanism with 44 species and about 120 reactions is derived from MELCHIOR [Derognat, 2003], following the concept of chemical operators [Carter, 1990]. This reduced mechanism is called MELCHIOR2 hereafter.

The CAMS CHIMERE version consists in the baseline gas-phase version with MELCHIOR2 chemistry, together with a sectional aerosol module. This module accounts for 7 species (primary particle material, nitrate, sulfate, ammonium, biogenic secondary organic aerosol SOA, anthropogenic SOA and water). Potentially, chloride and sodium can be included (high computing time). The aerosol distribution is represented using 9 bins from 10 nm to 10 µm.

2.3 Assimilation system

The CHIMERE assimilation for CAMS relies on a kriging based-approach to assimilate hourly concentration values for correcting the raw forecasts. This method has been widely evaluated and validated in the PREV'AIR (Rouïl et al, 2005) system for ozone and PM_{10}. However, future evolution of the CHIMERE assimilation system is foreseen to perform multi-pollutant and multi-sensor assimilation at the same time with a more complex method.

2.3.1 Kriging-based analysis

Several variants of kriging have been tested and compared (Malherbe et al., 2012): kriging of the innovations (i.e. kriging of CHIMERE errors); kriging with CHIMERE as external drift; ordinary co-kriging between the observations and CHIMERE.

- For operational applications, kriging with external drift, which gave the highest scores for ozone (Malherbe and Ung, 2009) and is faster than co-kriging, was found to be the best compromise between efficiency and computing time. It has been implemented in PREV'AIR since 2010, as replacement for kriging of the innovations. It proceeds according to the following steps:

Hourly monitoring data are retrieved from CAMS_50. Linear regression between a selected set of observations and CHIMERE is performed (in moving neighbourhood).

The experimental variogram of the regression residuals is computed and a variogram model is fitted; the model adequacy is checked by cross validation.

Observations are kriged with the CHIMERE model as external drift (in moving neighbourhood). Additional monitoring data, which are not used for calculating the variogram (e.g. data from some mountain sites), are included at this stage.

- For regulatory applications, the choice of the kriging technique and related parameters is adapted to each pollutant, according to cross-validation and validation tests:

For PM_{10} and $PM_{2.5}$, ordinary co-kriging of the observations (main variable) and CHIMERE (secondary variable) is currently applied.

For NO_2, kriging with external drift is performed.