CHIMERE 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	9
	Top altitude	500hPa
	Depth of lower most layer	20m
	Number of lower layers	7 below 2km
Initial & boundary conditions & meteorology	Meteorological driver	D-1 00:00 UTC IFS, 3hrly
	Boundary values	CAMS-Global IFS
	Initial values	Previous forecast
Emissions: natural & biogenic	In-domain soil and road dust emissions	Marticorena and Bergametti, 1995, (Menut et al, 2005).
	In-domain sea-salt emissions	Mårtensson et al. (2003), Monahan et al. (1986)
	Birch, Grass, Olive, Ragweed, Alder, Mugwort Pollen provided by FMI	yes
	Biogenic emissions	MEGAN V2.10 (Guenther et al., 2012)
	Soil NOx	MEGAN V2.10 (Guenther et al., 2012)
	Wildfiles 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	MELCHIOR2 (Derognat, 2003), 44 gaseous species and 120 reactions
	Heterogeneous chemistry	NO2, HNO3, N2O5
	Aerosol size distribution	10 bins from 10 nm to 40 µm
	Inorganic aerosols	thermodynamic equilibrium for the H+-NH4+-SO42--NO3--Na+-Cl--H2O system (ISORROPIA 2.1)
	Secondary organic aerosols	Bessagnet et al. (2009)
	Aqueous phase chemistry	SO2 oxidation
	Dry deposition: gases	resistance approach (Wesely, 1989)
	Dry deposition: aerosols	gravitational settling
	Wet deposition	In-cloud scavenging for all gas/aerosols is taken into account. Below cloud by rain and snow falls is taken into account for soluble gas (HNO3, H2O2) and particles
Assimilation	Assimilation method	Kriging-based analysis
	Assimilated surface pollutants	NO2, O3, PM2.5, PM10
	assimilated satellite	none
	Frequency of assimilation	Hourly

1.2 Model Overview

CHIMERE is a multi-scale CTM developed jointly by INERIS and CNRS (Mailler et al., 2017). Its development was initiated in the early 2000s (Vautard et al., 2005; Bessagnet et al., 2004; Menut, 2003) and it has since then pioneered operational national air quality forecasting in France (Rouïl et al., 2009) and it is also extensively used for long-term simulations for emission control scenarios (Colette et al., 2013; Meleux et al., 2007). It runs over a range of spatial scale from the hemispheric to the urban scale, with resolutions from 100km to 1km. The exact model version used as of June 2021 in the CAMS Regional Production is CHIMERE v2020r1 (Menut et al., 2021).

1.3 Model geometry

For the CAMS regional forecasts, CHIMERE uses a regular latitude-longitude grid with a 0.1°x0.1° resolution between 25˚W and 45˚E and 30˚N to 72˚N and 9 vertical levels, extending from the surface up to 500 hPa, a lowermost layer about 40m deep and about 7 layers below 2 km. No vertical downscaling is applied and concentrations in the lowermost model layer are considered representative of the surface.

1.4 Forcing Meteorology

The forcing meteorology is retrieved from the IFS model vertical layers covering the CHIMERE vertical extent on a 0.2°x0.2° horizontal grid resolution with a temporal resolution of 3 hours. The forecast released at 00:00UTC of the previous days is used. The meteorological parameters included to force the CHIMERE forecast are:
3D variables: horizontal wind components, temperature, specific humidity, orography, cloud liquid and ice water contents;
2D variables: surface temperature, surface pressure, total-low-medium-high cloud cover, cloud fraction, large scale and convective precipitations, rain water/snow mixing ratios, boundary layer height, sensible and latent heat fluxes at surface, surface solar radiation downwards, soil parameters (water and temperature) for 4 layers (0-7 cm, 7-28 cm, 28-100 cm, 100-255 cm), sea ice cover, snow depth.

1.5 Chemical initial and boundary conditions

Lateral and top boundary conditions are taken from chemical species available in the global IFS forecast model of the previous day at 3hr temporal resolution. The forecasts are initialised by the CHIMERE forecasts of the previous day.

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. Chemical disaggregation for VOCs is based on (Passant, 2002). PM components are speciated using the splits provided with the CAMS-REG database.
Biogenic VOC emissions are computed online with the MEGAN 2.10 algorithm (Guenther et al., 2012) implemented in CHIMERE and using high spatiotemporal data LAI (30 arcsec every 8 days) generated from MODIS (Yuan et al., 2011). Biogenic emission factors are estimated based on the 30 arcsec USGS (US Geophysical Survey) land-use database and the emission factors provided for each functional type by (Guenther et al., 2012).
The hourly GFAS wildfire emission for D-2 (i.e. the last full day available when launching the forecast system) are used for the analysis (D-1) and the first two days of the forecast (D+0 and D+1). Fire emissions are set to zero for the remainder of the forecast horizon.

Within domain mineral dust production schemes is included (Alfaro and Gomes 2001). It is based on a scheme for saltation and a vertical flux estimate using cohesion kinetic energies scheme (Marticorena and Bergametti, 1995) as well as additional numerical optimization (Menut et al, 2005).

1.7 Solver, advection and mixing

The numerical time solver is based on a splitting operator which solves separately transport (including deposition and emissions), chemistry and aerosol formation.
Advection is based on the Piecewise Parabolic Method 3d order scheme (Colella and Woodward, 1984). Vertical turbulent mixing takes place only in the boundary layer. The formulation uses K-diffusion parameterisation (Troen and Mahrt, 1986), without counter-gradient term.

1.8 Deposition

Dry deposition of gases species is parameterised as a downward flux out of the lowest model layer where the deposition velocity is described through a resistance analogy (Wesely, 1989). Wet deposition of particles and gases are computed by using a polydisperse distribution of rain droplets based on (Willis and Tattelman, 1989) and by computing the efficiency of the collision. Below-cloud scavenging of gases is assumed irreversible and is therefore only accounted for the most soluble compounds (HNO3, H2O2, HCl). In-cloud scavenging is accounted for all gases by computing the gaseous and aqueous phases partitioning based on Henry's law constants and the pH of the clouds. Scavenging by snow is also accounted for and is based on (Chang, 1984) for gases and on (Wang et al., 2014) for particles.

1.9 Chemistry and aerosols

In order to optimise computing time, the reduced MELCHIOR2 mechanism with 44 species and about 120 reactions is derived from MELCHIOR (Derognat, 2003). The sectional aerosol module accounts for 7 species and 10 bins from 10nm to 40µm (primary particle material, nitrate, sulphate, ammonium, biogenic secondary organic aerosol SOA, anthropogenic SOA and water). Photolytic rates are attenuated using liquid water or relative humidity. The aerosol module is described in great details in Couvidat et al. (2018) and accounts for condensation, nucleation, condensation/evaporation. Aerosol thermodynamic equilibrium is achieved using the ISORROPIA model version 2.1. The secondary organic aerosol formation mechanism is described in (Bessagnet et al., 2008).

1.10 Assimilation system

The CHIMERE assimilation for operational purposes relies on a kriging based-approach to assimilate hourly concentration values for correcting the raw model. For the analysis period, linear regression between a selected set of observations (excluding mountain and proximity sites) and the raw CHIMERE model is performed (in moving neighbourhood). The experimental variogram of the regression residuals is then computed and a variogram model is fitted; the model adequacy is checked by cross validation. Ultimately, observations are kriged with the CHIMERE model as external drift (in moving neighbourhood). This method is applied for O3 and NO2. For PM10 and PM2.5, an ordinary co-kriging of the observations (main variable) and

CHIMERE (secondary variable) is applied to ensure consistency between both pollutants. Only in-situ surface observations are used.
Further evolution of the CHIMERE assimilation system using an ensemble Kalman Filter approach is under development, in particular to pave the way for assimilation of satellite data. It is has however not yet demonstrated to provide better skill score than the geostatistical method.