# **LOTOS-EUROS Fact sheet**

## updated JUNE 2024

## 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	12
	Top altitude	200hPa
	Depth of lower most layer	8000 m
	Number of lower layers	45m
Initial & boundary	Meteorological driver	D-1 12:00 UTC IFS, 3hrly
conditions &	Boundary values	CAMS-Global IFS
meteorology	Initial values	Previous forecast
<b>Emissions:</b>	Inventory	CAMS-REG v6.1 REF2 2022
anthropogenic	Temporal disagregation	CAMS-REG-TEMPO_v4.1
Emissions: natural & biogenic	In-domain soil and road dust emissions	Marticorena and Bergametti (1995) and soil moisture inhibition as in Fécan et al. 1999
	In-domain sea-salt emissions	wind parameterisation of Monahan et al., 1986 and sea surface temperature (Martensson et al., 2003)
	Birch, Grass, Olive, Ragweed, Alder, Mugwort Pollen provided by FMI	yes
	Biogenic emissions	MEGAN (Guenther et al. 1993) with detailed tree types for Europe
	Soil NOx	Yienger and Levy (1995)
	Soil NOx Wildfiles emissions	Yienger and Levy (1995) Hourly emissions from D-2 cycled for AN (D-1) and FC (D+0 and D+1, zero for the remaining days)
	Soil NOx Wildfiles emissions Gas phase chemistry	Yienger and Levy (1995) Hourly emissions from D-2 cycled for AN (D-1) and FC (D+0 and D+1, zero for the remaining days) Modified CBM-IV
	Soil NOx Wildfiles emissions Gas phase chemistry Heterogeneous chemistry	Yienger and Levy (1995) Hourly emissions from D-2 cycled for AN (D-1) and FC (D+0 and D+1, zero for the remaining days) Modified CBM-IV Hydrolysis of N2O5
	Soil NOx Wildfiles emissions Gas phase chemistry Heterogeneous chemistry Aerosol size distribution	Yienger and Levy (1995) Hourly emissions from D-2 cycled for AN (D-1) and FC (D+0 and D+1, zero for the remaining days) Modified CBM-IV Hydrolysis of N2O5 5 size bins for dust and sea-salt, 2 size bins for other aerosols
Chemistry/	Soil NOx Wildfiles emissions Gas phase chemistry Heterogeneous chemistry Aerosol size distribution Inorganic aerosols	Yienger and Levy (1995) Hourly emissions from D-2 cycled for AN (D-1) and FC (D+0 and D+1, zero for the remaining days) Modified CBM-IV Hydrolysis of N2O5 5 size bins for dust and sea-salt, 2 size bins for other aerosols ISORROPIA-2
Chemistry/ Physics	Soil NOx Wildfiles emissions Gas phase chemistry Heterogeneous chemistry Aerosol size distribution Inorganic aerosols Secondary organic aerosols	Yienger and Levy (1995) Hourly emissions from D-2 cycled for AN (D-1) and FC (D+0 and D+1, zero for the remaining days) Modified CBM-IV Hydrolysis of N2O5 5 size bins for dust and sea-salt, 2 size bins for other aerosols ISORROPIA-2 not included
Chemistry/ Physics	Soil NOx Wildfiles emissions Gas phase chemistry Heterogeneous chemistry Aerosol size distribution Inorganic aerosols Secondary organic aerosols Aqueous phase chemistry	Yienger and Levy (1995) Hourly emissions from D-2 cycled for AN (D-1) and FC (D+0 and D+1, zero for the remaining days) Modified CBM-IV Hydrolysis of N2O5 5 size bins for dust and sea-salt, 2 size bins for other aerosols ISORROPIA-2 not included SO2 oxidation
Chemistry/ Physics	Soil NOx Wildfiles emissions Gas phase chemistry Heterogeneous chemistry Aerosol size distribution Inorganic aerosols Secondary organic aerosols Aqueous phase chemistry Dry deposition: gases	Yienger and Levy (1995) Hourly emissions from D-2 cycled for AN (D-1) and FC (D+0 and D+1, zero for the remaining days) Modified CBM-IV Hydrolysis of N2O5 5 size bins for dust and sea-salt, 2 size bins for other aerosols ISORROPIA-2 not included SO2 oxidation resistance approach (Erisman et al. 1994)
Chemistry/ Physics	Soil NOx Wildfiles emissions Gas phase chemistry Heterogeneous chemistry Aerosol size distribution Inorganic aerosols Secondary organic aerosols Aqueous phase chemistry Dry deposition: gases Dry deposition: aerosols	Yienger and Levy (1995) Hourly emissions from D-2 cycled for AN (D-1) and FC (D+0 and D+1, zero for the remaining days) Modified CBM-IV Hydrolysis of N2O5 5 size bins for dust and sea-salt, 2 size bins for other aerosols ISORROPIA-2 not included SO2 oxidation resistance approach (Erisman et al. 1994) Zhang (2001)
Chemistry/ Physics	Soil NOx Wildfiles emissions Gas phase chemistry Heterogeneous chemistry Aerosol size distribution Inorganic aerosols Secondary organic aerosols Aqueous phase chemistry Dry deposition: gases Dry deposition: aerosols Wet deposition	Yienger and Levy (1995) Hourly emissions from D-2 cycled for AN (D-1) and FC (D+0 and D+1, zero for the remaining days) Modified CBM-IV Hydrolysis of N2O5 5 size bins for dust and sea-salt, 2 size bins for other aerosols ISORROPIA-2 not included SO2 oxidation resistance approach (Erisman et al. 1994) Zhang (2001) Banzhaf et al. (2012)
Chemistry/ Physics	Soil NOx Wildfiles emissions Gas phase chemistry Heterogeneous chemistry Aerosol size distribution Inorganic aerosols Secondary organic aerosols Aqueous phase chemistry Dry deposition: gases Dry deposition: aerosols Wet deposition Assimilation method	Yienger and Levy (1995) Hourly emissions from D-2 cycled for AN (D-1) and FC (D+0 and D+1, zero for the remaining days) Modified CBM-IV Hydrolysis of N2O5 5 size bins for dust and sea-salt, 2 size bins for other aerosols ISORROPIA-2 Not included SO2 oxidation resistance approach (Erisman et al. 1994) Zhang (2001) Banzhaf et al. (2012)
Chemistry/ Physics	Soil NOx Wildfiles emissions Gas phase chemistry Heterogeneous chemistry Aerosol size distribution Inorganic aerosols Secondary organic aerosols Aqueous phase chemistry Dry deposition: gases Dry deposition: aerosols Wet deposition Assimilation method Assimilated surface pollutants	Yienger and Levy (1995) Hourly emissions from D-2 cycled for AN (D-1) and FC (D+0 and D+1, zero for the remaining days) Modified CBM-IV Hydrolysis of N2O5 5 size bins for dust and sea-salt, 2 size bins for other aerosols ISORROPIA-2 Not included SO2 oxidation resistance approach (Erisman et al. 1994) Zhang (2001) Banzhaf et al. (2012) ENKF NO2, O3, PM2.5, PM10
Chemistry/ Physics Assimilation	Soil NOx Wildfiles emissions Gas phase chemistry Heterogeneous chemistry Aerosol size distribution Inorganic aerosols Secondary organic aerosols Secondary organic aerosols Aqueous phase chemistry Dry deposition: gases Dry deposition: aerosols Wet deposition Assimilation method Assimilated surface pollutants assimilated satellite	Yienger and Levy (1995) Hourly emissions from D-2 cycled for AN (D-1) and FC (D+0 and D+1, zero for the remaining days) Modified CBM-IV Hydrolysis of N2O5 5 size bins for dust and sea-salt, 2 size bins for other aerosols ISORROPIA-2 Not included SO2 oxidation resistance approach (Erisman et al. 1994) Zhang (2001) Banzhaf et al. (2012) ENKF NO2, O3, PM2.5, PM10 NO2 (OMI)

## 1.2 Model Overview

The LOTOS-EUROS model is a 3D chemistry transport model aimed to simulate air pollution in the lower troposphere. The model has been used in a large number of studies for the assessment of particulate air pollution and trace gases (e.g. O3, NO2) (Hendriks et al., 2016; Schaap et al., 2013; Thürkow et al., 2021; Timmermans et al., 2022). A detailed description of the model is given in (Manders et al., 2017).

## 1.3 Model geometry

The domain of LOTOS-EUROS is the CAMS regional domain from 25°W to 45°E and 30°N to 72°N. The projection is regular longitude-latitude, at 0.1°x0.1° grid spacing. In the vertical and for the forecasts there are currently 12 model layers and 2 more reservoir layers at the top, defined by coarsening in a mass conservative way the first 77 model levels of the IFS. For the analyses there are 4 dynamic layers up to 5km agl and a surface layer with a fixed depth of 25 m. The lowest dynamic layer is the mixing layer, followed by 3 reservoir layers. The heights of the reservoir layers are determined by the difference between the mixing layer height and 5 km. For output purposes, the concentrations at measuring height (usually 2.5 m) are diagnosed by assuming that the flux is constant with height and equal to the deposition velocity times the concentration at height z. This applies for several of the gaseous species, namely O3, NO, NO2, HNO3, N2O5, H2O2, CO, SO2 and NH3. For aerosols, the same approach is utilised, only sedimentation velocity is used instead of deposition velocity.

## 1.4 Forcing Meteorology

The forcing meteorology is retrieved from the 00:00 and 12:00 UTC runs of the IFS model at hourly (surface fields) or 3-hourly temporal resolution (model layer fields). The meteorological data is retrieved on a regular horizontal resolution of about 15 km and for all layers covered by the model's vertical extent. The meteorological variables included are 3-hourly 3D fields for wind direction, wind speed, temperature, humidity and density, substantiated by hourly 2D gridded fields of mixing layer height, surface wind and temperature, precipitation rates, heat fluxes, cloud cover and surface variables snow depth, sea ice cover and volumetric soil water.

#### 1.5 Chemical initial and boundary conditions

The lateral and top boundary conditions for trace gases and aerosols are obtained from the CAMS-global daily forecasts. When the chemical boundary conditions from IFS are missing, the model uses climatological boundary concentrations derived from IFS data. The forecasts are initialized with the LOTOS-EUROS forecast of the previous day.

#### 1.6 Emissions

The common annual anthropogenic emissions CAMS-REG are implemented as explained in Section 2.6.1. Injection height distribution from the EuroDelta study is implemented, which is per SNAP (or more recently, GNFR) category. Time profiles used are defined per country

and GNFR emission category type. Time profiles from CAMS-TEMPO v4.1 can also be chosen for the distribution of the emissions over time.

Biogenic NMVOC emissions are calculated online using actual meteorological data and a detailed landuse and tree species database including emission factors from (Köble and Seufert, 2001). The isoprene emissions follow the mathematical description of the temperature and light dependence of the isoprene emissions, proposed by (Guenther et al., 1993). Sea salt emissions are parameterised following (Martensson et al., 2003; Monahan, 1986) from the wind speed at 10-meter height.

The fire emissions are taken from the near real-time GFAS fire emissions database. For the forecast, we assume persistence, so that the latest downloaded emission for the specific hour is used. When the hourly emission is more than 3 days old, it is set to zero.

Mineral dust emissions within the modelling domain are calculated online based on the sand blasting approach by (Marticorena and Bergametti, 1995) with soil moisture inhibition as described by (Fécan et al., 1998). Finally, a parameterization using land cover and temperature is used for handling soil NOx emissions, based on (Yienger and Levy, 1995).

### 1.7 Solver, advection and mixing

The transport consists of advection in 3 dimensions, horizontal and vertical diffusion, and entrainment/detrainment. The advection is driven by meteorological fields (u,v), which are input every 3 hours. The vertical wind speed w is calculated by the model as a result of the divergence of the horizontal wind fields. A linear advection scheme is used to ensure tracer mass conservation, which also allows more efficient parallelization and reduced model complexity. This scheme uses piece-wise linear functions to define sub-grid concentrations, which is sometimes referred to as MUSCL ("Monotonic Unwind-centered Scheme for Conservation Laws") following Van Leer (1977).

Vertical diffusion is described using the standard Kz theory. Vertical exchange is calculated employing the new integral scheme by (Yamartino et al., 2007). For the forecasting set-up with 12 layers, atmospheric stability values and functions, including Kz values, are derived based on the surface heat fluxes from ECMWF meteorology and similarity profiles following the IFS approach (ECMWF, 2021) to adapt for land-use specific conditions. For the 5-layer version in the assimilation, a correction is made for the vertical diffusion to correct for the height difference between surface and mixing layer.

#### 1.8 Deposition

The dry deposition in LOTOS-EUROS is parameterised following the resistance approach. The laminar layer resistance and the surface resistances for acidifying components are described following the EDACS system (Van Zanten et al., 2010), the deposition velocities for particles are based on (Zhang et al., 2001). Wet deposition is divided between in-cloud and below-cloud scavenging. The in-cloud scavenging module is based on the approach described in (Seinfeld and Pandis, 1998) and (Banzhaf et al., 2012).

#### 1.9 Chemistry and aerosols

LOTOS-EUROS uses the TNO CBM-IV scheme, which is a modified version of the original CBM-IV (Gery et al., 1989). LOTOS-EUROS uses a bulk approach for the aerosol size distribution differentiating between a fine and a coarse fraction, but for dust and sea salt there are 5 distinct size classes: ff: 0.1-1 $\mu$ m, f:1-2.5  $\mu$ m, ccc: 2.5-4  $\mu$ m, cc: 4-7  $\mu$ m, c:7-10  $\mu$ m. N2O5 hydrolysis is described explicitly based on the available (wet) aerosol surface area (using  $\gamma$  = 0.05) (Schaap et al., 2004). Aqueous phase and heterogeneous formation of sulfate is described by a simple first order reaction constant (Barbu et al., 2009; Schaap et al., 2004). Inorganic aerosol chemistry is represented using ISORROPIA II (Fountoukis and Nenes, 2007) and secondary organic aerosols formation based on a VBS scheme (Bergström et al., 2012b; Zare et al., 2014) will be included in the operational forecast version at the end of 2023.

#### 1.10 Assimilation system

The LOTOS-EUROS model is equipped with a data assimilation package with the ensemble Kalman filter technique (Curier et al., 2012). The ensemble is created by specification of uncertainties for emissions (NOx, VOC, NH3 and aerosol), ozone deposition velocity, and ozone top boundary conditions. Currently, data assimilation is performed for O3, NO2, PM10 and PM2.5 surface observations, OMI NO2 is also assimilated.

#### References

Leer, B. van, Towards the ultimate conservative difference scheme. IV. A new approach to numerical convection, Journal of Computational Physics, Volume 23, Issue 3, doi:10.1016/0021-9991(77)90095-X, 1977.