5. LOTOS-EUROS factsheet

5.1 Assimilation and forecast system: synthesis of the main characteristics

Assimilation and forecast system	
Horizontal resolution	0.1° (longitude) x 0.1° (latitude)
Vertical resolution	12 layers up to 100hPa for the forecasts and 5 layers with top at 5 km above sea level for the analyses
Gas phase chemistry	Modified version of the original CBM-IV
Heterogeneous chemistry	N_2O_5 hydrolysis
Aerosol size distribution	Bulk approach: $PM_{2.5}$ and $PM_{2.5-10}$
Inorganic aerosols	ISORROPIA-2
Secondary organic aerosols	Not included in this version
Aqueous phase chemistry	Linearized
Dry deposition/sedimentation	Resistance approach, following Erisman et al. (1994). Zhang (2001) deposition scheme is used for particles, explicitly including particle size and sedimentation
Mineral dust	Emissions after Marticorena&Bergametti (1995) with soil moisture inhibition as described by Fécan et al (1999)
Sea Salt	Parameterised based on wind speed at 10m following (Monahan et al., 1986) and sea-surface temperature (Martensson et al., 2003)
Boundary values	CAMS-global forecast (lateral and top)
Initial values	24h forecast from the day before
Anthropogenic emissions	CAMS-REG-AP_v4.2/2017
Biogenic emissions	Following Guenther et al. (1993) using 115 tree types over Europe
Forecast system	
Meteorological driver	12:00 UTC operational IFS forecast for the day before
Assimilation system	
Assimilation method	Ensemble Kalman filter
Observations	In-situ surface observations (O_3, NO_2, PM_{10}, $PM_{2.5}$) distributed by Meteo-France as well as OMI NO_2
Frequency of assimilation	Hourly, performed once a day for the previous day
Meteorological driver	00:00 UTC operational IFS forecast for the same day

5.2 Forward model

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. O_3, NO_2) (e.g. Manders et al. 2009, Hendriks et al, 2013, Curier et al, 2012, 2014, Schaap et al 2013). The model has participated frequently in international model comparisons addressing ozone (e.g. Solazzo et al. 2012a) and particulate matter (e.g. Solazzo et al. 2012b, Stern et al. 2008). For a detailed description of the model as well as for references not found in the references section of this document, we refer to Manders et al. (2017).

5.2.1 Model geometry

The domain of LOTOS-EUROS is the CAMS regional domain from 25°W to 45°E and 30°N to 70°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 and a surface layer. This version extends in the vertical up to 5 km above sea level. 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. Simulations incorporate a surface layer of a fixed depth of 25 m. 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 O_3, NO, NO_2, HNO_3, N_2O_5, H_2O_2, CO, SO_2 andNH_3. For aerosols, the same approach is utilized, only sedimentation velocity is used instead of deposition velocity.

5.2.2 Forcings and boundary conditions

5.2.2.1 Meteorology

The LOTOS-EUROS system in its standard version is driven by 3-hourly meteorological data. These include 3D fields for wind direction, wind speed, temperature, humidity and density, substantiated by 2D gridded fields of mixing layer height, precipitation rates, cloud cover and several boundary layer and surface variables. In CAMS, meteorological forecast data obtained from the ECMWF is used to force the model.

5.2.2.2 Chemistry

The lateral and top boundary conditions for trace gases and aerosols are obtained from the CAMS-global daily forecasts (see Table 5). As mentioned previously, LOTOS-EUROS uses a bulk approach for the aerosol size distribution differentiating between a fine and a course fraction but for dust and sea salt there are distinct, more detailed size classes, more specifically dust_ff, dust_f, dust_c, dust_cc, dust ccc, na_f, na_c, na_cc and na_ccc. The assumption as regards the diameters for those species are:_ff: 0.1-1 µm, _f:1-2.5 µm, ccc: 2.5-4 µm, _cc: 4-7 µm, _c:7-10 µm.

Table 5. The chemical and aerosol species taken from C-IFS and used in LOTOS-EUROS

CAMS-global Species	Coupled to LOTOS-EUROS Species	Comments
GO_3	O_3	
CO	CO	
NO	NO	
NO_2	NO_2	
PAN	PAN	
HNO_3	HNO_3	
HCHO	form	
SO_2	SO_2	
CH_4	CH_4	
C_5H_8	isop	
aermr01 (0.06-1 µm)	na_ff	Divided by 4.3 to reduce to dry sea salt
aermr02 (1-10 µm)	na_f, na_ccc, na_cc, na_c	Divided by 4.3 to reduce to dry sea salt. Distributed as follows: 10% to na_f, 20% to na_ccc, 40% to na_cc and 30% to na_c
aermr04 (0.06-1.1 µm)	dust_ff, dust_f	Distributed as follows: 20% to dust_ff and 80% to dust_f
aermr05 (1.1-1.8 µm)	dust_ff, dust_f	Distributed as follows: 20% to dust_ff and 80% to dust_f
aermr06 (1.8-40 µm)	dust_ccc, dust_cc, dust_c	Distributed as follows: 12% to dust_ccc, 24% to dust_cc, and 24% to dust_c
aermr07	ec_f	
aermr08	ec_f	
aermr09	pom_f	
aermr10	pom_f	
aerm11	so4a_f	
aerm16	no3a_f	
aerm17	no3a_c	
aerm18	nh4a_f	

When the dynamic boundaries from C-IFS are missing, the model uses climatological boundary concentrations derived from C-IFS data.

5.2.2.3 Land use

The land use is taken from the CORINE/Smiatek database enhanced with the 3 species map for Europe made by (Koeble and Seufert, 2001). The combined database has a resolution of 0.0166x0.0166°, which is aggregated, to the required resolution during the start-up of a model simulation.

5.2.2.4 Surface emissions

The anthropogenic emissions currently used are those of CAMS-REG-AP_v4.2/2017, which cover years 2000-2016 (Kuenen et al., 2014). From v1.8, the use of the stack 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. Biogenic isoprene emissions are calculated following the mathematical description of the temperature and light dependence of the isoprene emissions, proposed by (Guenther et al., 1993), using actual meteorological data. Sea salt emissions are parameterised following (Monahan et al., 1986) from the wind speed at 10-meter height. The fire emissions are taken from the near real-time GFAS fire emissions database.

Mineral dust emissions are calculated online based on the sand blasting approach by Marticorena&Bergametti (1995) with soil moisture inhibition as described by Fécan et al (1999). For wind speed, a roughness length of 0.013 m was used for bare soil, for the parameterisation of dust emissions a local (effective) roughness length of $8x10^{-4}$ m was used, with a smooth roughness length of $3x10^{-5}$ m. For the threshold friction velocity a tuning factor of 0.66 was used (Heinold et al (2007). The sandblasting efficiency was calculated according to Shao et al (1996). Soil characteristics were derived from the STATSGO maps based on the work by Zobler (1986) with USGS soil texture classes. A simple preferential sources map, based on topographical differences in a radius of 10 degrees, was derived following the approach by Ginoux et al (2001). In addition, a tuning constant of 0.5 was used to modify the total emission strength.

5.2.3 Dynamical core

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. The improved and highly accurate, monotonic advection scheme developed by (Walcek, 2000) is used to solve the system. The number of steps within the advection scheme is chosen such that the Courant restriction is fulfilled.

5.2.4 Physical parameterisations

5.2.4.1 Turbulence and convection

Entrainment is caused by the growth of the mixing layer during the day. Each hour the vertical structure of the model is adjusted to the new mixing layer depth. After the new structure is set, the pollutant concentrations are redistributed using linear interpolation. Vertical diffusion is described using the standard K_z theory. Vertical exchange is calculated employing the new integral scheme by (Yamartino et al., 2004).

Atmospheric stability values and functions, including Kz values, are derived using standard similarity theory profiles.

5.2.4.2 Deposition

The dry deposition in LOTOS-EUROS is parameterised following the well-known resistance approach. The laminar layer resistance and the surface resistances for acidifying components and particles are described following the EDACS system (Erisman et al., 1994). 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 (2006) and Banzhaf et al. (2012).

5.2.5 Chemistry and aerosols

LOTOS-EUROS uses the TNO CBM-IV scheme, which is a modified version of the original CBM-IV (Whitten et al., 1980). N_2O_5 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 sulphate is described by a simple first order reaction constant (Schaap et al., 2004; Barbu et al., 2009). Aerosol chemistry is represented using ISORROPIA II (Fountoukis, 2007).

5.3 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, NH_3 and aerosol), ozone deposition velocity, and ozone top boundary conditions. Currently, data assimilation is performed for O_3, NO_2, PM_{10} and $PM_{2.5}$, using surface observations collected and provided by Meteo-France each morning for the day before. OMI NO_2 is also assimilated.