8. SILAM factsheet

8.1 Assimilation and forecast system: synthesis of the main characteristics

Assimilation and forecast system	
Horizontal resolution	0.1° regular lat-lon grid
Vertical resolution	69 layers for meteorological pre-processor (IFS hybrid levels 69 to 137, covering the troposphere), 10 layers for chemistry and vertical sub-grid-scale mixing calculations, with layer tops at 25,75,175,375,775,1500,2700,4700,6700 and 8700m above surface
Gas phase chemistry	Modified CBM-5 gas-phase transformation, inorganic chemistry scheme with input to heterogeneous transformations (Sofiev, 2000)
Heterogeneous chemistry	Sofiev (2000)
Aerosol size distribution	Bins. Varies: for anthropogenic source, follows the emission of PM2.5-10 split, for sea salt uses 5 bins from 10nm up to 30μm, dust is split into 4 bins from 10nm up to 30 μm
Inorganic aerosols	SO4, NO3, NH4, EC, anthropogenic mineral, sea salt, desert dust
Secondary organic aerosols	Volatility Basis-Set
Aqueous phase chemistry	SO2 oxidation, nitrate formation (Sofiev, 2000), heterogeneous nitrate formation on sea salt particles
Dry deposition/sedimentation	Resistance approach (Wesely et al., 1989) for gases, (Kouznetsov & Sofiev, 2012) for aerosols
Mineral dust	Silam dust source
Sea Salt	Updated source term Sofiev et al (2011)
Boundary values	C-IFS values for all available species
Initial values	24h forecast from the day before
Anthropogenic emissions	CAMS-REG-AP_v4.2/2017
Biogenic emissions	Dynamic biogenic emissions, based upon Poupkou et al. (2010)
Forecast system	
Meteorological driver	12:00 UTC operational IFS forecast for the day before (up to +108)
Assimilation system	
Assimilation method	Operational intermittent 3d-var for analysis; 4dvar for pollen re-analysis
Observations	In-situ surface data O3, NO2, PM2.5, PM10, SO2, CO operational; and vertically integrated columns in

	research mode (NO2, AOD)
Frequency of assimilation	Hourly
Meteorological driver	00:00 UTC operational IFS forecasts up to +24h

8.2 Forward model

The System for Integrated modeLling of Atmospheric coMposition SILAM v.5.6 (Sofiev et al, 2015) is a Eulerian chemical transport model with the transport module based on advection scheme of Galperin (2000) refined by Sofiev et al (2015) and adaptive vertical diffusion algorithm of Sofiev (2002). Apart from the transport and physico-chemical cores described below, SILAM includes a set of supplementary tools including a meteorological pre-processor, input-output converters, reprojection and interpolation routines, etc. In the operational forecasts, these enabled direct forcing of the model by the ECMWF IFS meteorological fields. A system outlook can also be found at http://silam.fmi.fi.

8.2.1 Model geometry

8.2.1.1 Horizontal computational grid

number of grid cells: nx = 700 ny = 420
western-most longitude = 25.05 W, eastern-most longitude = 44.95° E
southern-most latitude = 30.05 N, northern-most latitude = 71.95° N
resolution: dx = 0.1° dy = 0.1°

8.2.1.2 Vertical grids

Following Sofiev (2002), SILAM uses a multi-vertical approach with the meteorology-resolving grid corresponding to the tropospheric part of the IFS vertical: hybrid levels from 69 to 137. The chemical transformations and vertical fluxes are computed based on 10 thick staggered layers, with the thickness increasing from 25 m for the lowest layer to 1000-2000 m in the free troposphere. Within the thick layers, the sub-grid information is used to evaluate the weighted averages of the high-resolution meteorological parameters and effective diffusion coefficients.

8.2.2 Forcings and boundary conditions

8.2.2.1 Meteorology

Meteorological forcing is the ECMWF IFS operational forecasts taken from the 12UTC forecast of the previous day. Thus, the forecast length of the meteorology fields is from +12 hr till +84 hr. The meteo fields are taken from the operational dissemination procedure of ECMWF in rotated lon-lat coordinates system (southern pole of the rotated grid is at (0E, 30S)) with 0.1° resolution.

8.2.2.2 Chemistry

Boundary conditions are taken from the C-IFS (see Table 8). The full fields are imported every 3 hours; in-between, the linear interpolation is applied. Due to repeated criticism of sea-salt levels of the IFS, the SSA boundary conditions are taken from SILAM own global forecasts.

Table 8. The chemical and aerosol species taken from C-IFS and used in SILAM

C-IFS Species	Coupled to SILAM Species	Comments
Go3	O3	Only GO3 is used by SILAM
CO	CO	
NO	NO	
NO2	NO2	
PAN	PAN	
SO2	SO2	
C5H8	C5H8	
C2H6	ETHA	
HNO3	HNO3	
Aermr04,"Dust Aerosol (0.03 - 0.55 um) Mixing Ratio" *	0.4xAermr04→ 0.3 um† dust mode, 0.6xAermr04 → 1.5um† dust mode	
Aermr05, "Dust Aerosol (0.55 - 0.9 um) Mixing Ratio"*	Aermr05 → 6um† dust mode	
Aermr06, "Dust Aerosol (0.9 - 20 um) Mixing Ratio"*	0.4xAermr06 → 6um† dust mode 0.6xAermr06 → 20 um† dust mode	
OC hydrophilic aermr07	AVB0	Non-volatile bin of organic aerosol
OC hydrophobic aermr08	AVB0	
BC hydrophilic aermr09	EC	

C-IFS Species	Coupled to SILAM Species	Comments
BC hydrophobic aermr10	EC	
Sulphates aermr 11	Sulphates	1 C-IFS mode split equally to 2 SILAM modes
Aermr01, "Sea Salt Aerosol (0.03 - 0.5 um) Mixing Ratio"*	0.232 x Aermr01 → 0.5um† sslt mode	Factor of 0.232 (1/4.3) used for conversion from wet to dry mass
Aermr02, "Sea Salt Aerosol (0.5 - 5 um) Mixing Ratio"*	0.232 x Aermr02 → 3um† sslt mode	Same as above
Aermr03, "Sea Salt Aerosol (5 - 20 um) Mixing Ratio"*	0.132 x Aermr01 → 9um† sslt mode 0.1 x Aermr01 → 20um† sslt mode	Same as above

* For aerosol sizes C_IFS uses wet radii
† For aerosol sizes Silam uses dry diameters

8.2.2.3 Surface emissions

Emission fields are based on the CAMS-REG-AP_v4.2/2017 database for CO, SO_2, NO_X, NH_3, NMVOC, $PM_{2.5}$ and $PM_{2.5-10}$, for reference year 2017. The $PM_{2.5}$ emissions are split into EC, OC and mineral components, and OC is mapped to the volatility bins according to Shrivastava et al.(2011). Emissions of biogenic VOCs and sea salt are computed in the corresponding SILAM dynamic modules, which are described below. GFAS hourly emissions from wild-land fires are replicated from D-2 to D+1 for forecast and shut down after, for analysis mode used as is.

8.2.3 Transport core

The SILAM Eulerian transport core (Sofiev et al, 2015) is based on the coupled developments: refined advection scheme of Galperin (2000) and vertical diffusion algorithm of Sofiev (2002) and Kouznetsov & Sofiev (2012). The methods are compatible, in a sense that both use the same set of variables to determine the sub-grid distribution of tracer mass. The approach, in particular, allows computing correct vertical exchange using high-resolution input data but low-resolution chemistry and diffusion grids. The later feature is used in the vertical setup with 10 thick layers.

8.2.4 Physical parameterisations

8.2.4.1 Turbulence and convection

Diffusion is parameterised following the first-order K-theory based closure. Horizontal diffusion is embedded into the advection routine, which itself has zero numerical viscosity, thus allowing full control over the diffusion fluxes. The vertical diffusivity parameterisation follows the approach suggested by Genikhovich et al. (2004), as described in Sofiev et al (2010). The procedure diagnoses all the similarity theory parameters using the profiles of the basic meteorological quantities: wind, temperature and humidity. Output includes the value of eddy diffusivity for scalars at some reference height (taken to be 1m).

8.2.4.2 Deposition

Dry deposition parameterisation follows the standard resistive analogy of Wesely (1989). Deposition velocity for aerosols are evaluated using the original (Kouznetsov & Sofiev, 2012) algorithm. Wet deposition parameterisation is based on the scavenging coefficient after Sofiev (2000) for gas species and a new deposition scheme for aerosols following the generalised formulations of (Kouznetsov & Sofiev, 2012).

8.2.5 Chemistry and aerosols

The main gas-phase chemical mechanism is CBM-5. The original CBM-5 scheme was transformed to avoid species that are a subset of other species (e.g. OLE includes PAR), to increas numerical stability of the scheme. The heterogeneous scheme is an updated version of the DMAT model scheme (Sofiev, 2000). It incorporates the formation pathways of secondary inorganic aerosols.

Emission of 2 sets of compounds is embedded into the simulations: biogenic VOC, sea salt, and desert dust. The bio-VOC computations follow the Poupkou et al. (2010) model and provide isoprene and mono-terpene emissions (currently, only isoprene emission is used in the CBM5 mechanism). The sea salt emission parameterisation is the original development generally based on Sofiev et al (2011), with refinements and spume formation mechanism added in v5.2.

8.3 Assimilation system

The embedded data assimilation is based on the 3- and 4-dimensional variational approach (3D-, 4D-VAR, Vira & Sofiev, 2012, 2015). The adjoint formulations exist for all dynamic modules, linearized transformation scheme of sulphur oxide and for aerosol particles. The assimilation procedure has been tested for both initialising the concentration fields and for refinement of the emission coefficients. The observation operators exist for in-situ observations and for the vertically integrated columns observed by the nadir-looking satellites.

For the near-real time analyses, the previous-day observations are used in a 3D-VAR data assimilation suite. The assimilated species are NO_2, O_3 and $PM_{2.5}$, PM_{10}, SO_2 and CO.