

# EURAD-IM Fact sheet

## 1.1 Assimilation and forecast system: synthesis of the main characteristics

<b>Discretisation</b>	Horizontal resolution	9x9 km Lambert conformal
	Number of vertical levels	23
	Top altitude	100hPa
	Depth of lower most layer	35m
	Number of lower layers	15 below 2km
<b>Initial &amp; boundary conditions &amp; meteorology</b>	Meteorological driver	D-1 12:00 UTC IFS for FC, IFS analysis for AN, 3hrly for FC, 6hrly for AN, downscaled with WRF
	Boundary values	CAMS-Global IFS
	Initial values	Previous forecast
<b>Emissions: natural &amp; biogenic</b>	In-domain soil and road dust emissions	Based on DREAM model
	In-domain sea-salt emissions	Sofiev et al. (2011)
	Birch, Grass, Olive, Ragweed, Alder, Mugwort Pollen provided by FMI	yes
	Biogenic emissions	MEGAN V2.10 (Guenther et al., 2012)
	Soil NO <sub>x</sub>	MEGAN V2.10 (Guenther et al., 2012)
	Wildfires emissions	last available 24h cycle over D-2 and D-1 cycled for AN (D-1) and FC (D+0 and D+1, zero for the remaining days)
<b>Chemistry/ Physics</b>	Gas phase chemistry	RACM-MM (Geiger et al., 2003)
	Heterogeneous chemistry	Hydrolysis of N <sub>2</sub> O <sub>5</sub>
	Aerosol size distribution	3 log-normal modes: 2 fine + 1 coarse
	Inorganic aerosols	thermodynamic equilibrium for the H <sup>+</sup> -NH <sub>4</sub> <sup>+</sup> -SO <sub>4</sub> <sup>2-</sup> -NO <sub>3</sub> <sup>-</sup> -H <sub>2</sub> O system (Friese and Ebel, 2010)
	Secondary organic aerosols	updated SORGAM module (Li et al., 2013)
	Aqueous phase chemistry	10 gas/aqueous phase equilibria, 5 irreversible S(IV) -> S(VI) transformations
	Dry deposition: gases	resistance approach (Zhang et al. 2003)
	Dry deposition: aerosols	resistance approach (Petroff and Zhang, 2010)
	Wet deposition	CMAQ (Roselle and Binkowski, 1999)
<b>Assimilation</b>	Assimilation method	Intermittent 3d-var
	Assimilated surface pollutants	NO <sub>2</sub> , O <sub>3</sub> , CO, SO <sub>2</sub> , PM <sub>2.5</sub> , PM <sub>10</sub>
	assimilated satellite	SO <sub>2</sub> columns from Aura/OMI
	Frequency of assimilation	Hourly

## 1.2 Model Overview

The EURAD-IM (European Air pollution Dispersion - Inverse Model) system consists of 5 major parts: the meteorological driver WRF, the pre-processors EEP and PREP for preparation of anthropogenic emission data and observations, the EURAD-IM Emission Model EEM, and the chemistry transport model EURAD (Hass et al., 1995, Memmesheimer et al., 2004). EURAD-IM

is a Eulerian meso-scale chemistry transport model involving advection, diffusion, chemical transformation, wet and dry deposition and sedimentation of tropospheric trace gases and aerosols. It includes 3d-var and 4d-var chemical data assimilation (Elbern et al., 2007) and is able to run in nesting mode.

### **1.3 Model geometry**

To cover the CAMS domain from 25°E to 45°W and 30°N to 72°N, two Lambert conformal projection subdomains with respectively 45 km (199x166 grid boxes) and 9 km horizontal resolution (581x481 grid boxes) are used. The model domain with the finer resolution covering the entire European part of the CAMS domain is nested within the halo domain with the coarser resolution.

Variables are horizontally staggered using an Arakawa C grid. Vertically, the atmosphere is divided by 23 terrain-following sigma coordinate layers between the surface and the 100 hPa pressure level. About 15 layers are below 2 km height. The thickness of the lowest layer is about 35 m. No vertical downscaling is used to derive surface concentrations from the first model level.

### **1.4 Forcing Meteorology**

The Weather Research and Forecast (WRF) model is used for the calculation of meteorological fields needed to drive the EURAD-IM CTM. Initial and boundary values for the WRF simulations are derived from IFS meteorological fields. The main motivation to use WRF is to improve the spatial and temporal interpolation of IFS fields towards the EURAD-IM geometry.

### **1.5 Chemical initial and boundary conditions**

The CAMS Global IFS 00:00 UTC forecast for the previous day is extracted from the MARS archive at ECMWF using 36 model levels with a temporal resolution of 3 hours. Use of Sea Salt from IFS using a scaling factor of 4.3 is under investigation.

### **1.6 Emissions**

The common annual anthropogenic emissions CAMS-REG are implemented as explained in Section 2.5. Temporal disaggregation is based on the GENEMIS tables (Ebel et al., 1997), using a GNFR to SNAP matrix. The VOC and PM split, the vertical distribution of area sources, and the emission strength per hour are calculated within the EURAD-IM CTM with the distribution profiles provided with the CAMS-REG-AP\_v4.2/2017 inventory (Kuenen et al., 2022). The VOC and PM split depends on source category and country, the vertical distribution only on the source category. For the temporal distribution of emissions monthly, weekly and daily profiles depending on source category are used.

Biogenic emissions and NO<sub>x</sub> emissions from soil are calculated within the EURAD-IM CTM with the Model of Emissions of Gases and Aerosols from Nature (MEGAN) (Guenther et al., 2012). Fire emissions are taken into account using hourly data from the Global Fire Assimilation System Version 1.2 (GFASv1.2) product (Kaiser et al., 2012). Zero fire emissions are assumed for D+2 and D+3 forecasts.

## **1.7 Solver, advection and mixing**

The positive definite advection scheme of Bott (1989), implemented in a one-dimensional realisation, is used to solve the advective transport. An operator splitting technique is employed (McRae, 1982) to handle the varying numerical specificities of processes to be solved.

An Eddy diffusion approach is used to parameterize the vertical sub-grid-scale turbulent transport. The calculation of vertical Eddy diffusion coefficients is based on the specific turbulent structure in the individual regimes of the planetary boundary layer (PBL) according to the PBL height and the Monin-Obukhov length (Holtslag and Nieuwstadt, 1986). A semi-implicit (Crank-Nicholson) scheme is used to solve the diffusion equation.

The sub-grid cloud scheme in EURAD-IM was derived from the cloud model in the EPA Models-3 Community Multiscale Air Quality (CMAQ) modelling system (Roselle and Binkowski, 1999). Convective cloud effects on both gas phase species and aerosols are considered.

## **1.8 Deposition**

The gas phase dry deposition modelling follows the method proposed by Zhang et al. (2003). Dry deposition of aerosol species is treated size dependent, using the resistance model of Petroff and Zhang (2010) with consideration of the canopy. Dry deposition is applied as lower boundary condition of the diffusion equation.

Wet deposition of gases and aerosols is derived from the cloud model in the CMAQ modelling system (Roselle and Binkowski, 1999). The wet deposition of pollen is treated according to Baklanov and Sorenson, 2001.

Size dependent sedimentation velocities are calculated for aerosol and pollen species. The sedimentation process is parameterized with the vertical advective transport equation and solved using the fourth order positive definite advection scheme of Bott (1989).

## **1.9 Chemistry and aerosols**

In the EURAD-IM CTM, the gas phase chemistry is represented by an extension of the Regional Atmospheric Chemistry Mechanism (RACM) (Stockwell et al., 1997) based on the Mainz Isoprene Mechanism (MIM) (Geiger et al., 2003). A 2-step Rosenbrock method is used to solve the set of stiff ordinary differential equations (Sandu and Sander, 2006). Photolysis frequencies are derived using the FTUV model (fast TUV) according to Tie et al. (2003). The radiative transfer model therein is based on the Tropospheric Ultraviolet-Visible Model (TUV) developed by Madronich and Weller (1990).

The modal aerosol dynamics model MADE (Ackermann et al., 1998) is used to provide information on the aerosol size distribution and chemical composition. To solve for the concentrations of the secondary inorganic aerosol components, a FEOM (fully equivalent operational model) version, using the HDMR (high dimensional model representation) technique (Rabitz et al., 1999, Nieradzik, 2005), of an accurate mole fraction based thermodynamic model (Friese and Ebel, 2010) is used. The updated SORGAM module (Li et al., 2013) simulates secondary organic aerosol formation.

## **1.10 Assimilation system**

The EURAD-IM assimilation system (Elbern et al., 2007) includes (i) the EURAD-IM CTM and its adjoint, (ii) the formulation of both background error covariance matrices for the initial states

and the emission, and their treatment to precondition the minimisation problem, (iii) the observational basis and its related error covariance matrix, and (iv) the minimisation including the transformation for preconditioning. The quasi-Newton limited memory L-BFGS algorithm described in Nocedal (1980) and Liu and Nocedal (1989) is applied for the minimisation. Currently assimilated in the EURAD-IM analysis and interim re-analysis are surface in-situ observations of O<sub>3</sub>, NO<sub>2</sub>, PM<sub>2.5</sub>, PM<sub>10</sub> and remote sensing data from several instruments: NO<sub>2</sub> and SO<sub>2</sub> column retrievals from Aura/OMI and MetOp/GOME-2, MOPITT CO profiles, and IASI CO partial columns.