4. EURAD-IM factsheet

4.1 Assimilation and forecast system: synthesis of the main characteristics

Assimilation and forecast system	
Horizontal resolution	9 km on a Lambert conformal projection
Vertical resolution	23 layers up to 100 hPa Lowest layer thickness about 35 m About 15 layers below 2 km
Gas phase chemistry	RACM-MIM
Heterogeneous chemistry	N_2O_5 hydrolysis: RH dependent parameterisation
Aerosol size distribution	3 log-normal modes: 2 fine + 1 coarse, fixed standard deviation
Inorganic aerosols	Thermodynamic equilibrium for the H^+-NH_4^+-SO_4^{2-}-NO_3^--H_2O system
Secondary organic aerosols	Updated SORGAM module
Aqueous phase chemistry	10 gas/aqueous phase equilibria 5 irreversible S(IV) -> S(VI) transformations
Dry deposition/sedimentation	Resistance approach/size dependent sedimentation velocity
Mineral dust	DREAM model
Sea Salt	Included
Boundary values	C-IFS forecast
Initial values	3d-var analysis for the previous day
Anthropogenic emissions	CAMS-REG-AP_v3.1/2016
Biogenic emissions	MEGAN V2.10 (Guenther et. al, 2012) Hourly GFAS wild fire emission data
Forecast system	
Meteorological driver	WRF forced by 12:00 UTC operational IFS forecast for the previous day
Assimilation system	
Assimilation method	Intermittent 3d-var
Observations	NRT surface in-situ data distributed by Meteo-France and INERIS, NO_2 and SO_2 column retrievals from Aura/OMI and MetOp/GOME-2, MOPITT CO profiles, IASI CO partial columns
Frequency of assimilation	Hourly
Meteorological driver	WRF forced by the operational IFS analysis for the previous day

4.2 Forward model

The EURAD-IM 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-IM (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.

4.2.1 Model geometry

To cover the CAMS domain from 25°E to 45°W and 30°N to 72°N, 2 Lambert conformal projections with 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.

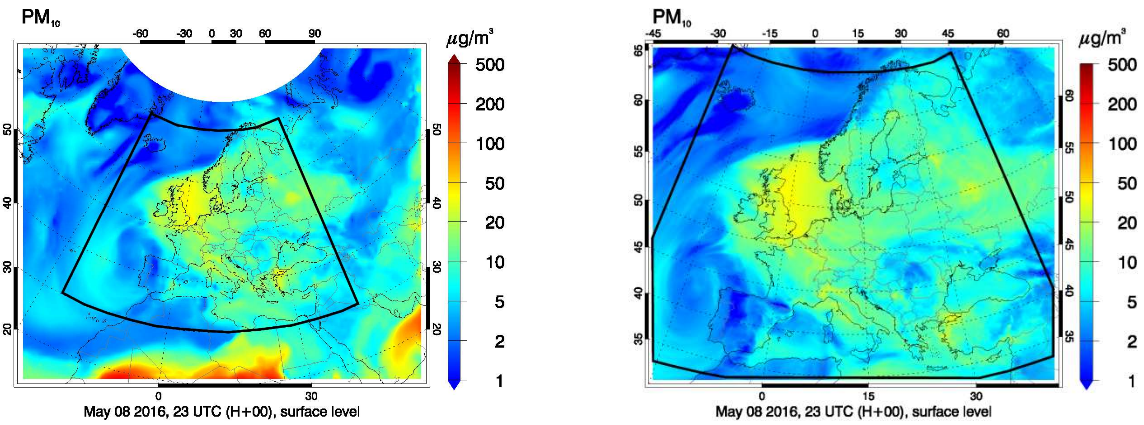

Figure 2 - EURAD-IM halo grid (left) and EURAD-IM nest with 15km horizontal resolution (right) used to cover the CAMS model domain (black line)

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. Both the EURAD-IM CTM and the WRF model use the same Lambert conformal projection and horizontal and vertical staggering of variables. No vertical downscaling is used to derive surface concentrations from the first model level.

4.2.2 Forcings and boundary conditions

4.2.2.1 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. Nudging of IFS data is not applied. The IFS operational 12:00 UTC forecast for the previous day is used for the provision of initial and boundary values for the WRF forecast. IFS data on 18 pressure levels between the surface and 30 hPa with a temporal resolution of 3 hours is horizontally and vertically interpolated by the WRF Pre-processing System (WPS). For the EURAD-IM air quality analysis, WRF simulations based on the operational IFS analysis for the times 00:00, 06:00, 12:00, and 18:00 UTC are used. For both the EURAD-IM forecast and analysis, hourly WRF output is temporally linearly interpolated within the EURAD-IM CTM to calculate meteorological variables at the transport time steps. EURAD-IM and WRF are using the same horizontal staggering of meteorological variables (Arakawa-C grid) on the same Lambert conformal projection. In addition both models use the same terrain following sigma coordinate. This enables a direct use of meteorological variables for the air quality simulation without additional horizontal and vertical interpolation steps. Mainly for this reason a calculation of meteorological fields with WRF is preferred to a direct use of IFS data.

4.2.2.2 Chemistry

For the provision of chemical gas phase and aerosol phase boundary values for the operational EURAD-IM air quality forecast and analysis, the C-IFS 00:00 UTC forecast for the previous day is directly extracted from the MARS archive at ECMWF (class=mc, expver=0001, type=fc). C-IFS data at 36 model levels with a temporal resolution of 3 hours is horizontally and vertically interpolated on the lateral boundaries of the halo domain with 45 km horizontal resolution used by the EURAD-IM CTM (see Table 4).

Use of Sea Salt from C-FIS using a scaling factor of 4.3 is under investigation.

Table 4. The chemical and aerosol species taken from C-IFS and used in EURAD-IM

C-IFS Species	Coupled to EURAD-IM Species	Comments
CO	CO	
C_2H_6	ETH	ethane
HCHO	HCHO	
HNO_3	HNO_3	
C_5H_8	ISO	isoprene
NO	NO	
NO_2	NO_2	

C-IFS Species	Coupled to EURAD-IM Species	Comments
GO_3	O_3	
PAN	PAN	
SO_2	SO_2	
Mineral dust	Mineral dust	95% coarse mode mineraldust, 5% accumulation mode mineraldust
Organic matter hydrophobic	Organic carbon	80% accumulation, 20% Aitken mode
Organic matter hydrophilic	Organic carbon	80% accumulation mode, 20% Aitken mode
Black carbon hydrophobic	Elemental carbon	70% accumulation mode, 30% Aitken mode
Black carbon hydrophilic	Elemental carbon	70% accumulation mode, 30% Aitken mode
Sulfate	SO_4	90% accumulation mode, 10% Aitken mode
Sea salt		Currently not used because of wet / dry mass discrepancy

4.2.2.3 Surface emissions

CAMS-REG-AP_v3.1/2016 is used for anthropogenic emissions. Yearly total emission amounts are area weighted horizontally interpolated on the EURAD-IM model grid. The VOC and PM split, the vertical distribution of area sources and the emission strength per hour is calculated within the EURAD-IM CTM based on profiles from the CAMS-REG-AP_v3.1/2016 inventory. For the vertical distribution of point sources profiles are taken partly from the EURAD-IM Emission Model (EEM) and partly from the CAMS-REG-AP_v3.1/2016 inventory. The VOC and PM split depends on source category and country, the vertical distribution only on source category. For the temporal distribution of emissions monthly, weekly and daily profiles depending on source category are used. Temporal profiles are shifted according to local time.
Biogenic emissions are calculated in the EURAD-IM CTM with the Model of Emissions of Gases and Aerosols from Nature (MEGAN) (Guenther et al., 2012). Emissions from fires are taken into account, using the Global Fire Assimilation System Version 1.2 (GFASv1.2) product (Kaiser et al., 2012) available daily with hourly temporal resolution at 0.1° x 0.1° horizontal resolution. Zero fire emissions are used for D+2 and D+3 forecasts. Emissions of birch, olive, grass, ragweed, and alder pollen are calculated within the EURAD-IM CTM dependent on meteorological conditions, according to algorithms provided by the FMI (Sofiev et al., 2015; Sofiev et al., 2017).

4.2.3 Dynamical core

To propagate a set of chemical constituents forward in time, the EURAD-IM CTM solves a system of partial differential equations:

$$\frac{\partial c_i}{\partial t} = -\nabla(\vec{v}\, c_i) + \nabla(\rho \mathbf{K} \nabla \frac{c_i}{\rho}) + A_i + E_i - S_i \, ,$$

where c_i is the mean mass mixing ratio of chemical species i, ***v*** are mean wind velocities, **K** is the eddy diffusivity tensor, ρ is air density, A_i is the chemical generation term for species i, E_i and S_i its emission and removal fluxes, respectively. The numerical solution of the above equation has its difficulties, due to the different numerical characters of the major processes. To overcome these problems an operator splitting technique is employed (McRae, 1982), wherein each process is independently treated in a sequence. The EURAD-IM CTM uses a symmetric splitting of the dynamical processes, encompassing the chemistry solver **C**:

$$c_i^{t+\Delta t} = T_h\, T_v\, D_v\, C\, D_v\, T_v\, T_h\, c_i^t,$$

where $T_{h,v}$ and D_v denote transport and diffusion operators in horizontal (h) and vertical (v) direction. The emission term is included in **C**.
The CTM's basic time-step Δt depends on the horizontal and vertical grid resolution in order to fulfil the CFL-criterion. If this criterion is locally not fulfilled, the time-step is dynamically adapted. $\Delta t_T = \Delta t/2$ is the transport time step used for the advection and diffusion with operators $T_{h,v}$ and D_v. For the gas phase chemistry calculations, the basic time step Δt is split into a set of variable time steps, which are often considerably smaller than Δt according to the chemical situation.

The positive definite advection scheme of Bott (1989), implemented in a one-dimensional realisation, is used to solve the advective transport.

4.2.4 Physical parameterisations

4.2.4.1 Turbulence and convection

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.

4.2.4.2 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).

4.2.5 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 differentials equations (Sandu and Sander, 2006). Photolysis frequencies are derived using the FTUV model 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.

4.3 Assimilation system

The EURAD-IM assimilation system 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) theminimisation 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.

The 3-dimensional variational data assimilation version of the EURAD-IM aims to minimise the following cost function:

$$J(\boldsymbol{x}) = \frac{1}{2}\left[\boldsymbol{x} - \boldsymbol{x}^{\mathrm{b}}\right]^{T} \mathbf{B}^{-1}\left[\boldsymbol{x} - \boldsymbol{x}^{\mathrm{b}}\right] + \frac{1}{2}\left[\boldsymbol{y} - H(\boldsymbol{x})\right]^{T} \mathbf{R}^{-1}\left[\boldsymbol{y} - H(\boldsymbol{x})\right]$$

with **x** being the current model state with background knowledge $\mathbf{x}^b$, H the observation operator, **B** the background error covariance matrix, **R** the observation error covariance matrix and **y** a set of observations. The minimum will be found by evaluating the gradient of the cost function with respect to the control variables **x**,

$$\nabla_{\boldsymbol{x}} J = \mathbf{B}^{-1}\left[\boldsymbol{x} - \boldsymbol{x}^{\mathrm{b}}\right] + \mathbf{H}^{T}\mathbf{R}^{-1}\left[\boldsymbol{y} - H(\boldsymbol{x})\right]$$

with $\mathbf{H}^T$ being the adjoint of the observation operator H. The observation operator is needed to get the model equivalent to each type of measurement, yielding the possibility to compare the model state to various kinds of observations. A powerful observation operator is implemented in the current version of the EURAD-IM data assimilation system, to assimilate heterogeneous sources of information like ground-based in-situ measurements as well as retrieval products of satellite observations, even using averaging kernel information.

Following Weaver and Courtier (2001) with the promise of a high flexibility in designing anisotropic and heterogeneous influence radii, a diffusion approach for providing **B** is implemented. Weaver and Courtier show that the diffusion equation serves as a valid operator for square-root covariance operator modelling by suitable adjustments of local diffusion coefficients. For a detailed description of the properties of the implemented background error covariance modelling, as well as the observation error covariance matrix **R**, see Elbern et al. (2007).

Currently assimilated in the EURAD-IM analysis and interim re-analysis are NRT surface in-situ observations of O_3, NO_2, $PM_{2.5}$, PM_{10} and remote sensing data from several instruments: NO_2 and SO_2 column retrievals from Aura/OMI and MetOp/GOME-2, MOPITT CO profiles, and IASI CO partial columns. Aircraft in-situ data for O_3, CO and NO_x from IAGOS are additionally assimilated in the validated re-analysis.