MONARCH Fact sheet

1.1 Assimilation and forecast system: synthesis of the main characteristics

Discretisation	Horizontal resolution	0.15° x 0.15° rotated regular lat-lon
	Number of vertical levels	24
	Top altitude	50hPa
	Depth of lower most layer	40m
	Number of lower layers	7 below 2km
Initial & boundary conditions & meteorology	Meteorological driver	D-1 12:00 UTC IFS, 6hrly, downscaled with NMMB
	Boundary values	CAMS-Global IFS
	Initial values	Previous forecast
Emissions: natural & biogenic	In-domain soil and road dust emissions	Mineral dust scheme based on Klose et al. (2021) and Pérez et al. (2011)
	In-domain sea-salt emissions	Jaeglé et al. (2011)
	Birch, Grass, Olive, Ragweed, Alder, Mugwort Pollen provided by FMI	yes
	Biogenic emissions	MEGAN v2.04 (Gunther et. al 2006)
	Soil NOx	MEGAN v2.04 (Gunther et. al 2006)
	Wildfiles emissions	Hourly emissions from D-2 cycled for AN (D-1) and FC (D+0 and D+1, zero for the remaining days)
Chemistry/ Physics	Gas phase chemistry	CB05 (Yarwood et al., 2005)
	Heterogeneous chemistry	Hydrolysis of N2O5 and aerosol uptake of HNO3 on dust and sea salt
	Aerosol size distribution	8 bins for dust and sea salt. Fine mode for BC, OM, SO4 and NH4. Coarse and fine mode for NO3
	Inorganic aerosols	EQSAM (Metzger et al., 2002)
	Secondary organic aerosols	non-volatile scheme for anthropogenic, biogenic and pyrogenic precursors (Pai et al., 2020)
	Aqueous phase chemistry	SO2 oxidation by ozone and H2O2
	Dry deposition: gases	resistance approach (Wesely, 1989)
	Dry deposition: aerosols	Zhang (2001) and Pérez et al. (2011)
	Wet deposition	Foley et al. (2010) and Pérez et al. (2011)
Assimilation	Assimilation method	LETKF Di Tomaso et al. (2017)
	Assimilated surface pollutants	NO2, O3, CO, SO2, PM2.5, PM10
	assimilated satellite	none
	Frequency of assimilation	Hourly

1.2 Model Overview

The MONARCH model is a fully online multiscale chemical weather prediction system for regional and global-scale applications (Pérez et al., 2011; Jorba et al., 2012; Badia and Jorba,

2015; Badia et al., 2017; Klose et al., 2021). The system is based on the meteorological Nonhydrostatic Multiscale Model on the B-grid (NMMB; Janjic and Gall, 2012), developed and widely verified at the National Centers for Environmental Prediction (NCEP). The model couples online the NMMB with the gas-phase and aerosol continuity equations to solve the atmospheric chemistry processes in detail. The model is designed to account for the feedbacks among gases, aerosol particles and meteorology. Currently, it can consider the direct radiative effect of aerosols while ignoring cloud–aerosol interactions.

1.3 Model geometry

The hybrid pressure-sigma coordinate is used in the vertical direction and the Arakawa B-grid is applied in the horizontal direction. The regional model is formulated on a rotated longitude–latitude grid, with the Equator of the rotated system running through the middle of the integration domain, resulting in more uniform grid distances. In the operational CAMS forecasts, the model is configured for a regional domain covering Europe and part of northern Africa with a regular horizontal grid spacing on the rotated projection of 0.15º (lower-left corner at 16.37ºN 22.14ºW, upper-right corner at 58.56ºN 88.18ºE) and the top of the domain is set at 50hPa using 24 vertical layers. Surface concentrations of gases and aerosols are derived directly from the first model level; no particular vertical downscaling is implemented. The depth of the first vertical layer of the model is around 45 m and about 7 layers are set below 2 km.

1.4 Forcing Meteorology

The forcing meteorology is retrieved from the IFS model on a 0.125°x0.125° horizontal grid resolution with a temporal resolution of 6 hours and dynamically interpolated to the final chemistry grid and time steps using the meteorological component of MONARCH. The IFS forecast released at 12:00UTC of the previous days is used. The meteorological variables obtained from IFS are: Skin temperature, Soil temperature, Soil moisture, Snow depth, Sea-ice mask, Sea-level pressure, U component of the wind, V component of the wind, Temperature, Geopotential height, Relative humidity or specific humidity, Cloud water content.

1.5 Chemical initial and boundary conditions

The variables used from chemical species available in the global IFS forecast mode are detailed in Table 2. Note that CH4 is not used from IFS because the MONARCH chemical mechanism considers a constant CH4 concentration of 1.85 ppmv. A remapping has been applied to couple the modal distribution of the IFS aerosols with the sectional distribution of the dust (0.2-0.36; 0.36-0.60; 0.60-1.20; 1.20-2.00; 2.00-3.60; 3.60-6.00; 6.00-12.00; 12.00-20.00µm) and sea salt (0.10-0.18; 0.18-0.30; 0.30-0.60; 0.60-1.00; 1.00-1.80; 1.80-3.00; 3.00-6.00; 6.00-15.00µm) aerosols of the MONARCH model. The forecasts are initialised by the model results of the previous day.

1.6 Emissions

The common annual anthropogenic emissions CAMS-REG are implemented as explained in Section 3.2. The High-Elective Resolution Modelling Emission System version 3 (HERMESv3; (Guevara et al., 2019) is used to pre-process the anthropogenic and biomass burning emissions

for the MONARCH model. HERMESv3 is an open source, parallel and stand-alone multiscale atmospheric emission modelling framework that processes gaseous and aerosol emissions for use in atmospheric chemistry models.
CAMS_REG-AP NMVOC and PM2.5 emissions are speciated using the sector and country-dependent split factors proposed by TNO. In terms of NOx, a fraction of 90% NO and 10% NO2 is considered for all sectors except for road transport, in which the following fractions are applied: (i) 95% NO, 4.2% NO2 and 0.8 HONO for gasoline road transport and (ii) 70% NO, 28.3% NO2 and 1.7% HONO for diesel road transport (Rappenglück et al., 2013). The vertical distribution of anthropogenic emissions is performed following the sector-dependent profiles proposed by TNO. The temporal distribution follows the CAMS-TEMPO v3.2 profiles (Guevara et al., 2021).
The biogenic emissions for NMVOC and NO are computed on-line within the MONARCH model using the Model of Emissions of Gases and Aerosols from Nature version 2.04 (MEGANv2.04; (Guenther et al., 2006). MEGAN is able to estimate the net emission rate of gases and aerosols from terrestrial ecosystems into the above-canopy atmosphere. MEGAN canopy-scale emission factors differ from most other biogenic emission models, which use leaf-scale emission factors and cover more than 130 NMVOCs. All the MEGAN NMVOCs are speciated following the CB05 chemical mechanism used in MONARCH; thus, emissions for isoprene, lumped terpenes, methanol, acetaldehyde, ethanol, formaldehyde, higher aldehydes, toluene, carbon monoxide, ethane, ethene, paraffin carbon bond, and olefin carbon bond are considered within the model. Soil NOx emissions are obtained from MEGAN.
Finally, biomass burning emissions (forest, grassland and agricultural waste fires) of organic carbon, black carbon, SO2, and Dimethylsulfide are taken from the GFASv1.3 dataset. This product reports hourly emissions at a horizontal gridded resolution of 0.1° x 0.1°. The vertical allocation of GFAS emissions is done using the maximum fire plume injection height and distributing uniformly all the emissions across the layers below this height. The persistence of the fires in forecast mode is set to 2 days, afterwards biomass burning emissions are set to zero.

1.7 Solver, advection and mixing

Different chemical processes were implemented following a modular operator splitting approach to solve the advection, diffusion, emission, dry and wet deposition, and chemistry processes. In order to maintain consistency with the meteorological solver, the chemical species are advected and mixed at the corresponding time step of the meteorological tracers following the principles described in Janjic an Gall (2012) and references therein. The advection scheme is Eulerian, positive definite and monotone, maintaining a consistent mass conservation of the chemical species within the domain of study. Lateral diffusion is formulated following the Smagorinsky non-linear approach, while vertical diffusion is based on the Mellor–Yamada–Janjic level 2.5 turbulence closure scheme.
The convective mixing, however, is treated differently for aerosols and gases. The scheme implemented for aerosols is described in detail in Pérez et al. (2011) and follows a relaxation approach similar to the Betts-Miller-Janjic convective parameterization of the NMMB. On the other hand, the convective mixing of gases is solved following the sub-grid cloud scheme of Byun and Ching (1999) and Foley et al. (2010) as described in Badia et al. (2017).

1.8 Deposition

The deposition processes implemented in the MONARCH model are dry deposition, in-cloud grid-scale, and in-cloud subgrid-scale scavenging for gases and aerosols, and below cloud scavenging for aerosols only.
For gases, the dry deposition scheme follows the classical deposition velocity analogy, enabling the calculation of deposition fluxes from airborne concentrations. The canopy resistance is simulated following Wesely (1989). The cloud-chemistry processes are included in the system considering both sub-grid and grid-scale processes following Byun and Ching (1999) and Foley et al. (2010). The processes included are the scavenging, vertical mixing and wet-deposition. Only in-cloud scavenging is considered in the current implementation (Badia et al., 2017).
Regarding aerosols, the parameterization of the aerosol dry deposition is based on Zhang et al. (2001) which includes simplified empirical parameterizations for the deposition processes of Brownian diffusion, impaction, interception and gravitational settling. Aerosol rebound at the surface is not taken into account due to limited knowledge of this process. Wet scavenging of aerosols by precipitation is computed separately for convective and grid-scale (stratiform) precipitation. It represents the most efficient process for the deposition of the smallest particles. The model includes parameterizations for in-cloud scavenging, and for below cloud scavenging. Detailed description of the schemes can be found in Pérez et al. (2011).

1.9 Chemistry and aerosols

A gas-phase module combined with a hybrid sectional-bulk mass-based aerosol module is implemented in the MONARCH model. The gas-phase chemical mechanism used is the Carbon Bond 2005 chemical mechanism (CB05; Yarwood et al., 2005) extended with Chlorine chemistry (Sarwar et al., 2012). The CB05 is well formulated for urban to remote tropospheric conditions. It considers 51 chemical species and solves 156 reactions, and the rate constants were updated based on evaluations from Atkinson et al. (2004) and Sander et al. (2006). The photolysis scheme used in the MONARCH model is the Fast-J scheme (Wild et al., 2000). It is coupled with physics of each model layer (e.g., aerosols, clouds, absorbers as ozone) and it considers grid-scale clouds from the atmospheric driver.
The aerosol module in MONARCH model solves the life cycle of sea salt, dust, organic matter (both primary and secondary), black carbon, sulfate, and nitrate aerosols. While a sectional approach is used for dust and sea salt, a bulk description of the other aerosol species is adopted. A simplified gas–aqueous–aerosol mechanism accounts for sulfur chemistry (Spada, 2015). The production of secondary nitrate–ammonium aerosol is solved using the thermodynamic equilibrium model EQSAM (Metzger et al., 2002). The coarse nitrate production is computed with an uptake reaction of HNO3 on dust and sea salt coarse particles. The formation of SOA is considered using a simple non-volatile scheme accounting for the contribution of anthropogenic, biomass burning, and biogenic formation (Pai et al., 2020). Mineral dust emissions can be calculated online using one of the schemes described in Pérez et al. (2011) and Klose et al. (2021), while several source functions are available to compute sea salt aerosol emissions (Spada et al., 2013). Hygroscopic growth is considered for all aerosol components except mineral dust.

1.10 Assimilation system

The MONARCH assimilation system (MONARCH-DA) is based on a Local Ensemble Transform Kalman Filter (LETKF) scheme (Hunt et al., 2007; Miyoshi and Yamane, 2007; Schutgens et al., 2010; Di Tomaso et al., 2017; Escribano et al., 2022) coupled to the model through I/O routines. MONARCH ensemble is created by perturbing anthropogenic, biomass burning, soil and ocean emissions that are pre-processed by HERMESv3 or that are modelled by MONARCH via a physically-based scheme for dust aerosol. The former are obtained by applying bidimentional multiplicative noise (constant in the vertical, in time and across species) extracted from a lognormal distribution (mean 1, standard deviation 0.5), and with a longitude and latitude correlation scale set to 10 grid points. Perturbations of dust emission parameters are analogous to those in Di Tomaso et al. (2022) but for the six ensemble members used for the operational analysis production. For analysis production in CAMS, MONARCH ensemble is run at a horizontal resolution of 0.2° latitude × 0.2° longitude in a rotated grid and initialised by the ensemble forecast of the previous day.

Hourly surface observations from in-situ measurements are currently assimilated operationally for O3, NO2, SO2, CO, PM10, PM2.5. The species are assimilated independently without cross-species covariance. We have assumed a linear model for the characterization of observation uncertainty for each species, and a diagonal observation error covariance matrix, i.e. uncorrelated error between the different measurements. For near-real time operational analysis production, previous-day observations are combined with a MONARCH 24-hour ensemble forecast initialised at 12 UTC of the previous day.

Within the LETKF algorithm the analysis at each model grid point can be calculated independently, and at each grid point only observations within a certain distance are assimilated. We have set this distance to 15 grid points from each analysis location. Additionally, spatial covariance localization is performed in the observation error covariance matrix, making the influence of an observation on the analysis decay gradually towards zero as the distance from the analysis location increases. To achieve this, the observation error is divided by a distance-dependent function that decays to zero with increasing distance, i.e. e^{-dist^2/l^2}, where dist is the distance in the grid space between an observation and the model grid and l is a spatial localization factor. Similarly, a temporal localization is applied to limit the influence of an observation in time. While observations are considered for assimilation at each hour, due to the 4D extension of the implemented LETKF scheme, observations affect the whole assimilation window (24 hours). The horizontal localization factor was set to 5, which makes the observation influence practically fade to zero before 10 model grid points away from the observation location (in the horizontal plane), while the vertical localization factor was set to 8 and the temporal localization factor was set to 3. Additionally, for in-situ observations, the vertical extension of the observation influence is limited to a maximum model level (currently set to level 12). The above localization settings are fixed independently of the species and geographical location.