Documentation of the MONARCH regional system and report on the development activities

October 2018 to April 2019

Issued by: METEO-FRANCE

Date: 03/05/2019

Ref:

CAMS50\_2018SC1\_D2.2.1.MONARCH-P1\_201906\_Dvpt\_report\_v0.1

This document has been produced in the context of the Copernicus Atmosphere Monitoring Service (CAMS).

The activities leading to these results have been contracted by the European Centre for Medium-Range Weather Forecasts, operator of CAMS on behalf of the European Union (Delegation Agreement signed on 11/11/2014). All information in this document is provided "as is" and no guarantee or warranty is given that the information is fit for any particular purpose.

The user thereof uses the information at its sole risk and liability. For the avoidance of all doubts, the European Commission

and the European Centre for Medium-Range Weather Forecasts has no liability in respect of this document, which is merely representing the authors view.

Contributors

BSC

O. Jorba

D. Bowdalo

D. Chmielewska

M. Guevara

M-T. Pay

C. Perez Garcia-Pando  
H. Petetin

INERIS

A. Colette

METEO-FRANCE

G. Collin

N. Assar

Table of Contents

[1. MONARCH factsheet 6](#_Toc7768526)

[1.1 Assimilation and forecast system: synthesis of the main characteristics 6](#_Toc7768527)

[1.2 Forward model 7](#_Toc7768528)

[1.2.1 Model geometry 7](#_Toc7768529)

[1.2.2 Forcing and boundary conditions 7](#_Toc7768530)

[1.2.2.1 Meteorology 7](#_Toc7768531)

[1.2.2.2 Chemistry and aerosols 7](#_Toc7768532)

[1.2.2.3 Surface emissions 8](#_Toc7768533)

[1.2.3 Dynamical core 8](#_Toc7768534)

[1.2.4 Physical parameterisations 8](#_Toc7768535)

[1.2.4.1 Turbulence and convection 8](#_Toc7768536)

[1.2.4.2 Deposition 8](#_Toc7768537)

[1.2.5 Chemistry and aerosols 8](#_Toc7768538)

[1.2.5.1 Chemistry 8](#_Toc7768539)

[1.2.5.2 Aerosol 8](#_Toc7768540)

[2. MONARCH development activities performed between October 2018 and April 2019 9](#_Toc7768541)

[2.1 Setting-up of the forecasts over the CAMS domain 9](#_Toc7768542)

[2.2 Any other development 9](#_Toc7768543)

[3. MONARCH development activities planned to be performed between May and October 2019 10](#_Toc7768544)

[3.1 Introduction of required input data (emission, meteorology, boundary conditions) 10](#_Toc7768545)

[3.2 Any other development 10](#_Toc7768546)

[4. References 11](#_Toc7768547)

Executive summary

The Copernicus Atmosphere Monitoring Service (CAMS, [atmosphere.copernicus.eu/](file:///\\petra1.meteo.fr\ACCES_AUTORISES\CAMS\SC1%20Deliverables\Compiled%20deliverables\Qr.%20daily%20analyses,%20forecasts,%20verification%20-%2003%20-%20MAM2016\Final\A%20livrer\atmosphere.copernicus.eu\)) is establishing the core global and regional atmospheric environmental service delivered as a component of Europe's Copernicus programme. The Regional forecasting service (CAMS\_50) currently provides daily 4-day forecasts of the main air quality species and analyses of the day before, as well as posteriori re-analyses using the latest validated observation dataset available for assimilation.

A median ENSEMBLE is computed based on the outputs of individual state-of-the-art atmospheric chemistry models, since ensemble products yield on average better performance. In addition to the 7 models already taking part in the operational production, 2 models are planned to join the pool of operational models in the very short term. Moreover, CAMS\_50 has expanded to include 2 new partners in view of further extending the number of models contributing to the ENSEMBLE at a later stage: the models they operate are referred to as “candidate models”.

This report documents the MONARCH regional forecasting and analysis system that is one of the candidate models. The development activities performed from October 2018 to April 2019 are described as well as their validation. The MONARCH developments planned for the period from May to October 2019 are also outlined.

During the period, the main achievements were: (1) the set up of the CAMS\_50 regional European domain, (2) the upgrade of the MONARCH preprocessing tools to digest the IFS forecast files for meteorology initial and boundary conditions, (3) the upgrade of the MONARCH preprocessing tools to digest the C-IFS forecast files for gases and aerosols boundary conditions, and (4) the processing of CAMS emissions. The HERMESv3\_gr model, used as the emission preprocessor of the MONARCH model, has been configured and executed to process the CAMS-REG-v2.2.1 and CAMS-GLOB datasets to provide the anthropogenic, soil and ocean emission fluxes over the MONARCH CAMS\_50 domain. Currently, the GFAS emissions used are the daily dataset. Further developments regarding the GFAS hourly emissions are pending to the availability of this dataset for the year 2016.

# MONARCH factsheet

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

|  |  |
| --- | --- |
| **Assimilation and forecast system** | |
| Horizontal resolution | 0.2º x 0.2º or 0.1º x 0.1º |
| Vertical resolution | 48 hybrid pressure-sigma vertical levels with the top of the atmosphere at 50 hPa |
| Gas phase chemistry | CB05 with extended Tu and Cl chemistry |
| Heterogeneous chemistry | Hydrolisis of N2O5 |
| Aerosol size distribution | 8 sectional bins for dust and sea salt, and bulk modes for organic matter, black carbon, sulfate, nitrate and ammonium |
| Inorganic aerosols | sulfate, nitrate and ammonium |
| Secondary organic aerosols | Two product scheme for isoprene and monoterpenes |
| Aqueous phase chemistry | sulfate aqueous formation |
| Dry deposition/sedimentation | Wesely (1989) resistance approach for gases and Zhang et al. (2001) for aerosols / sedimentation as described in Pérez et al. (2011) |
| Mineral dust | Pérez et al. (2011) emission scheme with further updates |
| Sea Salt | Several open-ocean emission schemes available (Spada et al., 2013). No surf-zone emissions. |
| Boundary values | Values provided by CAMS |
| Initial values | 24h forecast from the day before |
| Anthropogenic emissions | CAMS-REG-v2.2.1 and CAMS-GLOB datasets to cover the whole MONARCH domain |
| Biogenic emissions | MEGAN |
| Pollens | None |
| Assimilation module | Only for dust (Di Tomaso et al., 2017) |
| **Forecast system** | |
| Meteorological driver | Nonhydrostatic Multiscale Model on the B grid (NMMB) with IFS initial and boundary conditions. |

## Forward model

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, 2014; Badia et al., 2017). 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 En- vironmental 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.

Different chemical processes were implemented following a modular operator splitting approach to solve the advection, diffusion, chemistry, dry and wet deposition, and emission processes. Meteorological information is available at each time step to solve the chemical 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 using the same numerical schemes implemented in the NMMB. The advection scheme is Eulerian, positive definite and monotone, maintaining a consistent mass conservation of the chemical species within the domain of study (Janjic et al., 2009; Tang et al., 2009; Janjic and Gall, 2012).

### 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.

### Forcing and boundary conditions

#### Meteorology

The pre-processor of the MONARCH model can handle a wide range of forcing meteorological conditions to prepare the initial and boundary meteorological conditions for the NMMB. The list of meteorological inputs compatible with MONARCH is the following:

* GFS analysis and forecast data from the NCEP
* FNL final analysis data from the NCEP
* ERA-Interim reanalysis data from the ECMWF
* ERA5 reanalysis data from the ECMWF
* MERRA2 reanalysis data from the NASA

The pre-processor requires at least the following meteorological variables:

* 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

#### Chemistry and aerosols

The pre-processor of the MONARCH model has been upgraded to properly digest the C-IFS (CAMS) forecast data and prepare the gas and aerosol boundary conditions. The variables used from C-IFS are detailed in Table 1. Note that CH4 is not used from C-IFS because the MONARCH chemical mechanism considers a constant CH4 concentration.

Table 1. The chemical and aerosol fields taken from C-IFS and used in MONARCH.

| **C-IFS Species** | **Coupled to MONARCH Species** |
| --- | --- |
| var4: Dust Aerosol (0.03 - 0.55 um) Mixing Ratio\_kgkg-1 | remapped to the corresponding dust bins |
| var5: Dust Aerosol (0.55 - 0.9 um) Mixing Ratio\_kgkg-1 | remapped to the corresponding dust bins |
| var6: Dust Aerosol (0.9 - 20 um) Mixing Ratio\_kgkg-1 | remapped to the corresponding dust bins |
| var1: Sea Salt Aerosol (0.03 - 0.5 um) Mixing Ratio\_kgkg-1 | remapped to the corresponding sea salt bins |
| var2: Sea Salt Aerosol (0.5 - 5 um) Mixing Ratio\_kgkg-1 | remapped to the corresponding sea salt bins |
| var3: Sea Salt Aerosol (5 - 20 um) Mixing Ratio\_kgkg-1 | remapped to the corresponding sea salt bins |
| var8: Hydrophobic Organic Matter Aerosol Mixing Ratio\_kgkg-1 | primary hydrophobic organic matter |
| var7: Hydrophilic Organic Matter Aerosol Mixing Ratio\_kgkg-1 | primary hydrophilic organic matter |
| var10: Hydrophobic Black Carbon Aerosol Mixing Ratio\_kgkg-1 | hydrophobic black carbon |
| var9: Hydrophilic Black Carbon Aerosol Mixing Ratio\_kgkg-1 | hydrophilic black carbon |
| var11: Sulphate Aerosol Mixing Ratio\_kgkg-1 | sulphate |
| var121: NO2\_kgkg-1 | NO2 |
| var27: NO\_kgkg-1 | NO |
| var203: O3\_kgkg-1 | O3 |
| var6: HNO3\_kgkg-1 | HNO3 |
| var124: CH2O\_kgkg-1 | FORM (Formaldehyde) |
| var123: CO\_VMR | CO |
| var13: PAN\_kgkg-1 | PAN |
| var122: SO2\_kgkg-1 | SO2 |

A remapping has been applied to couple the modal distribution of the C-IFS aerosols with the sectional distribution of the dust and sea salt aerosols of the MONARCH model. The remapping implemented for mineral dust considers the size distribution in emission and is the following:

* MONARCH dust bin1 (0.2-0.36 m) = CAMS var4 x 0.17
* MONARCH dust bin2 (0.36-0.6 m) = CAMS var4 x 0.83
* MONARCH dust bin3 (0.6-1.2 m) = CAMS var5 x 1.
* MONARCH dust bin4 (1.2-2 m) = CAMS var6 x 0.03
* MONARCH dust bin5 (2-3.6 m) = CAMS var6 x 0.11
* MONARCH dust bin6 (3.6-6 m) = CAMS var6 x 0.22
* MONARCH dust bin7 (6-12 m) = CAMS var6 x 0.49
* MONARCH dust bin8 (12-20 m) = CAMS var6 x 0.15

In the MONARCH model, the sea salt aerosol is transported as dry matter using an 8 bin sectional distribution. To formulate the remapping, we consider that the reported sea salt mixing ratios out of global CAMS are for 80% relative humidity. To transform the provided values back to dry matter a reduction factor of 4.3 is needed for the mass mixing ratios and a reduction factor of 1.99 for the radii of the sea salt bin limits. The remapping implemented for sea salt is the following:

* MONARCH sea salt bin1 (0.1-0.18 m) = CAMS var1 x 0.34
* MONARCH sea salt bin2 (0.18-0.3 m) = CAMS var1 x 0.30 + CAMS var2 x 0.02
* MONARCH sea salt bin3 (0.3-0.6 m) = CAMS var2 x 0.13
* MONARCH sea salt bin4 (0.6-1 m) = CAMS var2 x 0.18
* MONARCH sea salt bin5 (1-1.8 m) = CAMS var2 x 0.35
* MONARCH sea salt bin6 (1.8-3 m) = CAMS var2 x 0.32 + CAMS var3 x 0.06
* MONARCH sea salt bin7 (3-6 m) = CAMS var3 x 0.40
* MONARCH sea salt bin8 (6-15 m) = CAMS var3 x 0.54

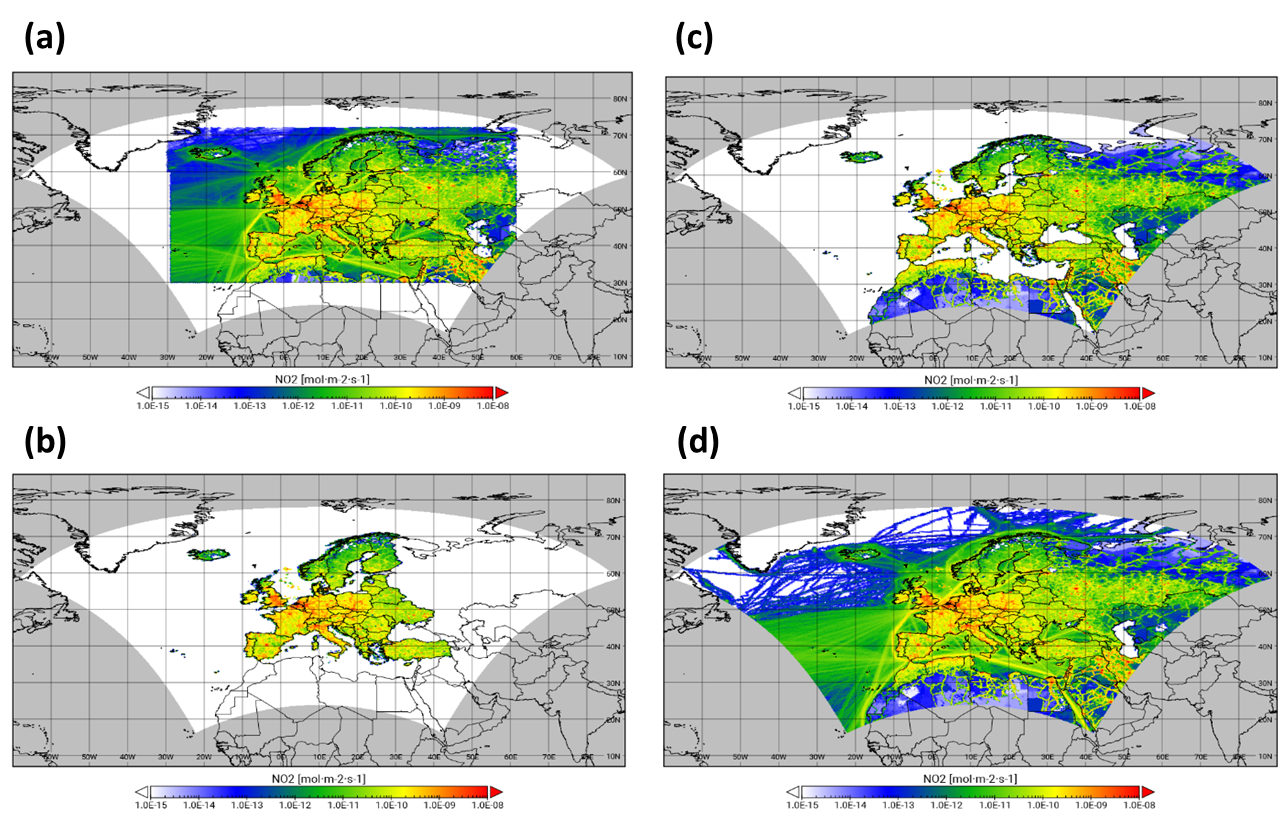
These remappings may be slightly modified during the first year of the project after analyzing the results of the model using this first implementation.

#### Surface emissions

The High-Elective Resolution Modelling Emission System version 3 (HERMESv3; Guevara et al., 2019) is used to pre-process the anthropogenic, biomass burning, soil and ocean 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.. The user can flexibly define combinations of existing up-to-date global and regional emission inventories and apply country specific scaling factors and masks. Each emission inventory is individually remapped onto the desired destination grid and processed using user-defined vertical, temporal and speciation profiles that allow obtaining emission outputs compatible with multiple chemical mechanisms. The selection and combination of emission inventories and databases is done through detailed configuration files.

We use HERMESv3 to process the CAMS\_REG-APv2.2.1 (all sectors except for shipping) and CAMS\_GLOB-APv2.1- anthropogenic emissions (all sectors except for shipping), the CAMS\_GLOB-SHIPv1.1 shipping emissions, the CAMS\_GLOB-SOILv1.1 and CAMS\_GLOB-OCEANv1.1 soil and ocean emissions and GFASv1.2 biomass burning emissions for the MONARCH CAMS\_50\_PhaseII domain.

The CAMS\_REG-APv2.2.1 dataset is applied to the 31 EEA countries and 4 EU candidate countries, while the CAMS\_GLOB-APv2.1 is used for all the other countries included in the MONARCH CAMS\_50\_PhaseII domain. The combination of both inventories was needed to avoid having regions of the MONARCH CAMS\_50\_PhaseII domain not covered (Figure 1a). Similarly, the CAMS\_GLOB-SHIPv1.1 emissions are used to ensure that all the maritime emissions that affect the MONARCH CAMS\_50\_PhaseII domain are included (Figure 1d).



**Figure 1 Representation of the anthropogenic emissions used in the MONARCH CAMS\_50\_PhaseII domain: original CAMS\_REG-APv2.2.1 emissions (a), CAMS\_REG-APv2.2.1 only in the countries completely covered (i.e. 31 EEA countries and 4 EU candidate countries) (b), inclusion of CAMS\_GLOB-APv2.1 to the rest of the countries (c) and inclusion of CAMS\_GLOB-SHIPv1.1 shipping emissions (d).**

All the criteria pollutants (i.e. NOx, NMVOC, CO, SO2, NH3, PM10, PM2.5) included in the CAMS\_REG-APv2.2.1, CAMS\_GLOB-ANTv2.1 and CAMS\_GLOB-SHIPv1.1 inventories are used. CAMS\_REG-APv2.2.1 and CAMS\_GLOB-SHIPv1.1 NMVOC and PM2.5 emissions are speciated using the sector and country dependent split factors proposed by TNO (the PM split factor file was recently updated due to the bug detected in the C\_OtherStationaryCombustion sector). CAMS\_GLOB-APv2.1 NMVOCs are already provided following the 25 GEIA VOCs groups and with the organic and black carbon fractions of PM2.5. 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 (Rappenglueck et al., 2013).

Vertical and temporal distribution of anthropogenic emissions is performed following the sector-dependent profiles proposed by TNO. We are currently running sensitivity test simulations using the new CAMS gridded temporal profiles that are currently being developed under CAMS81.

For CAMS\_GLOB-OCEANv1.1 only DMS emissions are used. Original monthly emissions are distributed assuming a flat daily and diurnal profile. For CAMS\_GLOB-SOILv1.1 NOx emissions are assumed to be 100% NO. Original monthly emissions are distributed assuming a flat daily profile and a diurnal profile based on temperature diurnal evolution. In the current runs, no canopy factor corrections are applied to the original emissions. We are planning to run sensitivity test simulations using different canopy correction factors, following the recommendations of CAMS81.

The biogenic emissions 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 non-methane volatile organic compounds (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. Biogenic emissions are computed every hour to account for evolving meteorological changes in solar radiation and surface temperature. Thus, the weather-driving variables considered are temperature at 2m and incoming shortwave radiation at the surface. NO MEGAN biogenic emissions are currently switched off as they are being considered with the CAMS\_GLOB-SOILv1.1 dataset. Sensitivity runs to compare the results obtained with CAMS\_GLOB-SOILv1.1 and MEGAN will be performed.

Finally, biomass burning emissions (forest, grassland and agricultural waste fires) of organic carbon, black carbon, SO2, and Dimethylsulfide are taken from the GFASv1.2 dataset (Kaiser et al., 2012). This product reports daily emissions at a horizontal gridded resolution of 0.1° x 0.1°. Although the requirements of CAMS\_50\_PhaseII specifies the use of hourly GFAS emissions, these are not available for the year of study where the MONARCH model will be evaluated (2016) yet. The vertical allocation of GFAS emissions is done using the maximum fire plume injection height derived from Sofiev et al. (2013) and distributing uniformly all the emissions across the layers below this height.

Currently, no lightning or volcano emissions are considered.

### Dynamical core

The dyamical core of the MONARCH model is the Nonhydrostatic Multiscale Model on the B-grid (NMMB; Janjic and Gall, 2012). The NMMB was conceived for short- and medium-range forecasting over a wide range of spatial and temporal scales, from large eddy simulations (LES) to global simulations. Its unified nonhydrostatic dynamical core allows for running of either regional or global simulations, both including embedded regional nests. The NMMB has been developed within the Earth System Modeling Framework (ESMF) at NCEP, following the general modeling philosophy of the NCEP regional Weather Research and Forecasting (WRF) Nonhydrostatic Mesoscale Model (NMM; Janjic, 2003). The regional NMMB has been the operational regional North American Mesoscale (NAM) model at NCEP since October 2011. Isotropic horizontal finite volume differencing is employed so that a variety of basic and derived dynamical and quadratic quantities are conserved. Among these, the conservation of energy and enstrophy improves the accuracy of the non-linear dynamics. The nonhydrostatic component of the model dynamics is introduced through an add-on module that can be turned on or off, depending on the resolution (Janjic et al., 2001).

### Physical parameterisations

#### Turbulence and convection

The operational physical package of the NMMB includes (1) the Mellor–Yamada–Janjic (MYJ) level 2.5 turbulence closure for the treatment of turbulence in the planetary boundary layer (PBL) and in the free atmosphere, (2) the surface layer scheme based on the Monin–Obukhov similarity theory with an introduced viscous sublayer over land and water, (3) the NCEP NOAH land surface model for the computation of the heat and moisture surface fluxes, (4) the RRTMG longwave and shortwave radiation package, (5) the Ferrier grid-scale clouds and microphysics, and (6) the Betts–Miller–Janjic convective parametrization. Vertical diffusion is handled by the surface layer scheme and by the PBL scheme. Lateral diffusion is formulated following the Smagorinsky non-linear approach.

Both gases and aerosols experience turbulence and convective mixing during their life cycle in the atmosphere. In MONARCH, the turbulence mixing of chemical species is solved with the same numerical scheme implemented in the NMMB. 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 in MONARCH is solved following the sub-grid cloud scheme of the CMAQ and RADMv2.6 model as described in Badia et al. (2016).

#### 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 aerodynamic resistance (Ra; depends only on atmospheric conditions) and the quasilaminar sublayer resistance (Rb; depends on friction velocity and modelcular characteristics of gases) are computed following their common definition, while the canopy or surface resistance (Rc) is simulated following Wesely (1989), where Rc is derived from the resistances of the surfaces of the soil and the plants. The properties of the plants are determined using land-use data (from the land use of the meteorological driver) and depend on the season. The surface resistance also depends on the diffusion coefficient, the reactivity, and the water solubility of the reactive trace gases. 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 detailed in Slinn (1982). 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).

### Chemistry and aerosols

#### Chemistry

A flexible gas-phase module is implemented in the MONARCH model. Currently, the Carbon Bond 2005 chemical mechanism (CB05; Yarwood, 2005) extended with Toluene and Chlorine chemistry is the default scheme of the model. Two options for solving the gas-phase chemistry are implemented: (1) an efficient and fast solver based on the Euler-Backward-Iterative shceme, and (2) a chemical mechanism and chemistry solver based on the Kinetic PreProcessor KPP package with the main purpose of maintaining a wide flexibility when configuring the model. The CB05 is well formulated for urban to remote tropospheric conditions and it considers 51 chemical species and solves 156 reactions. Both the organic chemistry of methane and ethane, and the chemistry of methylperoxy radical, methyl hydroperoxide and formic acid are treated explicitly. The higher organic peroxides, organic acids, and peracids are treated as lumped species. Following its main design, CB05 defines proxy single and double carbon bond species, paraffin and an olefin bond, respectively, and it introduces the internal olefin species. The rate constants were updated based on evaluations from Atkinson et al. (2004) and Sander et al. (2006). Organic compounds not explicitly treated are apportioned to the carbon-bond species based on the molecular structure and following Yarwood et al. (2005) assignments from VOC species to CB05 model species. The concentration of methane is considered constant (1.85 ppm) in the mechanism.

The photolysis scheme used in the MONARCH model is the Fast-J scheme. 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 Fast-J scheme has been updated with CB05 photolytic reactions. The quantum yields and cross section for the CB05 photolysis reactions have been revised and updated following the recommendations of Atkinson et al. (2004) and Sander et al. (2006). The Fast-J scheme uses seven different wavelength bins appropriate for the troposphere to calculate the actinic flux covering from 289 to 850 nm. Currently, aerosols are not considered in the photolysis rate calculation. This might produce an atmosphere excessively oxidized in regions where aerosols are significant.

#### Aerosol

The aerosol scheme of the MONARCH model follows a hybrid sectional-bulk multicomponent approach. The scheme extends from the seminal work of Pérez et al. (2011) that coupled on-line a state-of-the-art mineral dust module within the NMMB model. The system was upgraded with the implementation of 4 new aerosols in Spada et al. (2013) and Spada (2015) and currently describes the life cycle of mineral dust, sea-salt, black carbon, organic matter (both primary and secondary), sulfate, nitrate, and ammonium aerosols. While a sectional approach is used for mineral dust and sea-salt, a bulk description of the other aerosol species is adopted. A simplified gas-aqueous-aerosol mechanism has been introduced in the module to account for the sulfur chemistry. The EQSAM thermodynamic equilibrium model is used to solve the production of secondary inorganic nitrate and ammonium. And two options are available to estimate to formation of secondary organic aerosol: (1) a two-product scheme with isoprene and monoterpene precursor formation, and (2) a simple non-volatile scheme accounting for the contribution of anthropogenic, biomass burning, and biogenic formation.

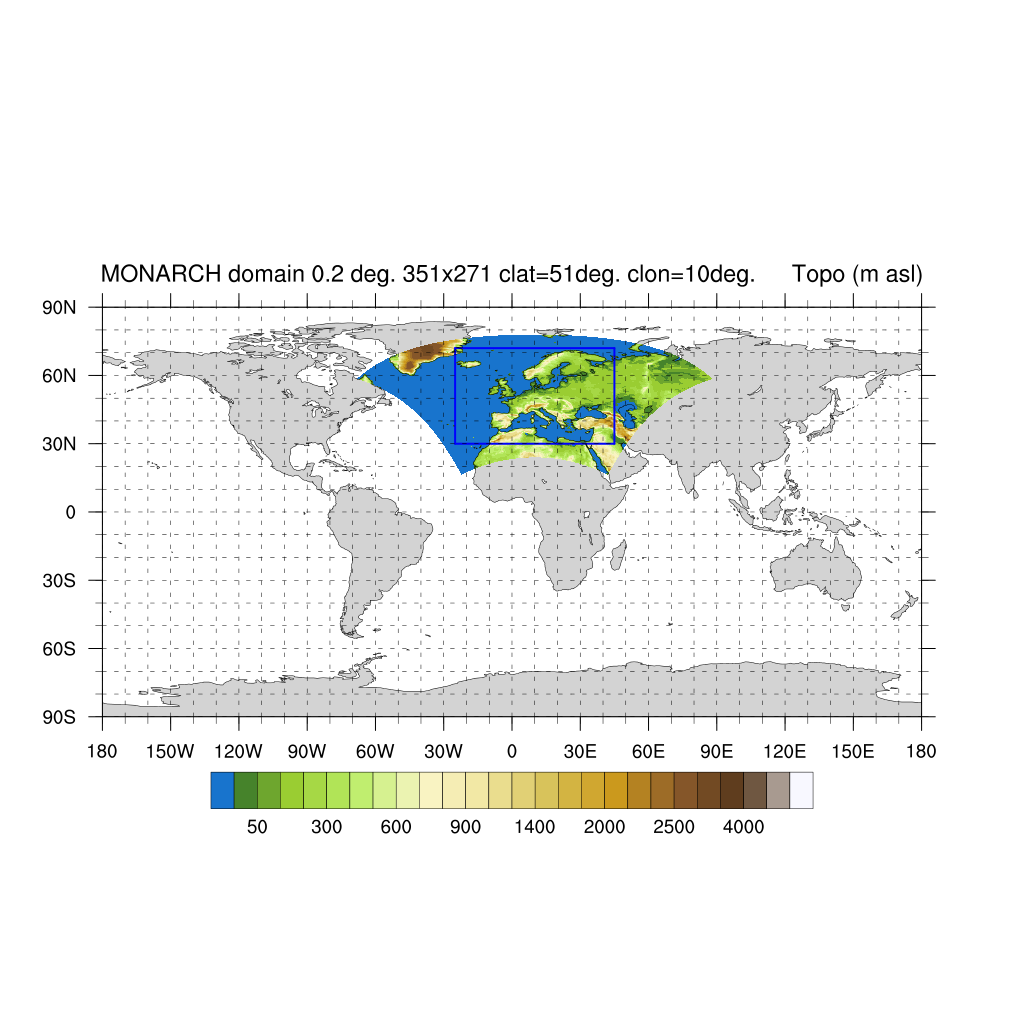
Mineral dust is treated as an hydrophobic particle, sea salt as hydrophilic, both black carbon and primary organic aerosol are emitted as hydrophobic particles and an aging process transforms them to hydrophilic, secondary organic aerosol (SOA) is considered hydrophilic, and sulfate/nitrate/ammonium are treated as a hydrophilic particles.

# MONARCH development activities performed between October 2018 and April 2019

## Setting-up of the forecasts over the CAMS domain

* Development activities to adapt the system over the European CAMS domain:

The MONARCH model uses a rotated latitude-longitude projection for limited area configurations. The domain designed to fulfil the CAMS\_50\_PhaseII requirements is shown in Figure 2. The CAMS\_50\_PhaseII requirements specifies that the model results should cover at least the domain 25°W-45°E, 30°N-72°N at a resolution finer or equal to 0.2°. To cover 72°N, the MONARCH domain has to be much larger than the requested area. Two different horizontal resolutions are under test during the first year of the CAMS\_50\_PhaseII project: (1) 0.1° x 0.1° and (2) 0.2° x 0.2°.



**Figure 2. The MONARCH domain covering the requested domain of the CAMS\_50\_PhaseII project. The Blue square covers the CAMS\_50\_PhaseII area.**

The vertical coordinate of the MONARCH model is a hybrid pressure-sigma coordinate. The model is configured with 48 vertical layers and a top of the atmosphere at 50 hPa. The transition from sigma to pressure is set at 300 hPa.

* Development activities to process emissions for CAMS50:

We use HERMESv3 to process the CAMS\_REG-APv2.2.1 (31 EEA countries and 4 EU candidate countries and all sectors except for shipping) and CAMS\_GLOB-APv2.1- anthropogenic emissions (rest of countries and all sectors except for shipping), the CAMS\_GLOB-SHIPv1.1 shipping emissions, the CAMS\_GLOB-SOILv1.1 and CAMS\_GLOB-OCEANv1.1 soil and ocean emissions and GFASv1.2 biomass burning emissions for the MONARCH CAMS\_50\_PhaseII domain. The sector and country dependent NMVOC and PM split factors proposed by TNO are being used. Vertical and temporal distribution of anthropogenic emissions is performed following the sector-dependent profiles proposed by TNO. Currently running a sensitivity test simulation using the new CAMS gridded temporal profiles that are currently being developed under CAMS81.

* Development activities to process IFS forecast meteorological data for CAMS50:

The pre-processor of the MONARCH model has been upgraded to properly digest the IFS forecast data and prepare the meteorological initial and boundary conditions. The fields used from IFS are:

* Skin temperature
* Soil temperature at 0-7cm, 7-28 cm, 28-100 cm and 100-255 cm
* Soil moisture at 0-7cm, 7-28 cm, 28-100 cm and 100-255 cm
* Snow depth
* Sea-ice mask
* Sea-level pressure
* U component of the wind
* V component of the wind
* Temperature
* Geopotential height
* Relative humidity

Currently, the IFS pressure level files are selected and downloaded from the MARS database due to downloading time constraints. In the future, we plan to explore the impact of working with the IFS sigma level files.

The IFS data is re-projected from the spectral and regular reduced latitude-longitude grid to a regular latitude-longitude grid. The latter format is the one compatible with the MONARCH pre-processor.

* Development activities to process C-IFS forecast gas and aerosol data for CAMS50:

The pre-processor of the MONARCH model has been upgraded to properly digest the C-IFS (CAMS) forecast data and prepare the gas and aerosol boundary conditions. The variables used from C-IFS are detailed in Table 1. Note that CH4 is not used from C-IFS because the MONARCH chemical mechanism considers a constant CH4 concentration.

* Development activities to simulate the Forecast experiment for CAMS50:

We have downloaded the IFS and C-IFS data for the Forecast experiment. The time period for this short forecast is 20160826 (D+0) to 20160829 (D+3).

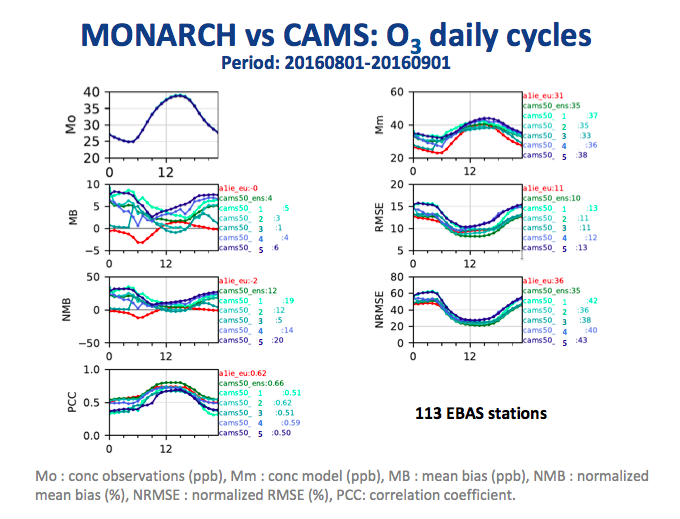
* Development activities to simulate the Hindcast experiment for CAMS50:

We have downloaded the complete year 2016 of C-IFS data for the Hindcast experiment. The IFS data is currently being downloaded.

## Any other development

* Evaluation activities

Evaluation activities are ongoing to assess the performance of the model with the new developments required by the CAMS\_50\_PhaseII project. The model has been evaluated with EIONET and EBAS observations of O3 and NO2 working with the CAMS\_50\_PhaseII domain, CAMS81 emissions, C-IFS boundary conditions, and GFS initial and boundary conditions. Figure 3 shows results of an evaluation of summer 2016 for O3.



**Figure 3. Preliminary O3 evaluation of the MONARCH model for August 2016 using CAMS\_50\_PhaseII domain, CAMS81 emissions, C-IFS boundary conditions, and GFS meteorological initial and boundary conditions. The MONARCH results are in red, the CAMS50 ensemble in dark green, and individual CAMS50 models in other colours.**

# MONARCH development activities planned to be performed between May and October 2019

## Introduction of required input data (emission, meteorology, boundary conditions)

* GFAS hourly emissions

Currently, we work with GFASv1.2 daily emission fluxes. During the next six months we plan to implement the treatment of GFASv1.2 hourly emission dataset in the HERMESv3 model and in the MONARCH model. A specific methodology for the temporal profiles and vertical injection of the emissions will be implemented.

* Forecast simulation

## Any other development

During the next six months we plan to improve the PM of the model. We envisage the five main tasks:

* Evaluation activities with EIONET, EBAS and AERONET observations
* Select the best mineral dust emission scheme for the CAMS\_50\_PhaseII domain and fine tune the remapping of the CAMS BC mineral dust and the MONARCH sectional dust
* Select the best sea salt emission scheme for the CAMS\_50\_PhaseII domain and fine tune the remapping of the CAMS BC sea salt and the MONARCH sectional sea salt
* Fine tune of the heterogeneous hydrolysis of N2O5 for the CAMS\_50\_PhaseII requirements
* Upgrade of the SOA scheme to deal with anthropogenic, biogenic, and biomass burning precursors, and associated aging processes

# References

Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., and Troe, J.: Evaluated kinetic and photochemical data for atmospheric chemistry: Volume I - gas phase reactions of Ox, HOx, NOx and SOx species, *Atmos. Chem. and Phys.*, 4, 1461–1738 (2004).

Badia, A., Jorba, O., Voulgarakis, A., Dabdub, D., Pérez García-Pando, C., Hilboll, A., Gonçalves, M., and Janjic, Z. Description and evaluation of the Multiscale Online Nonhydrostatic AtmospheRe CHemistry model (NMMB-MONARCH) version 1.0: Gas-phase chemistry at global scale. *Geosci. Model Dev.*, 10, 609-638 (2017).

Badia, A. and Jorba, O. Gas-phase evaluation of the online NMMB/BSC-CTM model over Europe for 2010 in the framework of the AQMEII-Phase2 project. *Atmos. Environ.*, 115, 657- 669 (2015)

Byun, D. and Ching, J.: Science algorithms of the EPA Models-3 community multiscale air quality (CMAQ) modeling system, Rep.EPA/600/R-99, 30 (1999).

Di Tomaso, E., Schutgens, N.A.J., Jorba, O., and C. Pérez García-Pando. Assimilation of MODIS Dark Target and Deep Blue observations in the dust aerosol component of NMMB- MONARCH version 1.0. *Geosci. Model Dev.*, 10, 1107-1129 (2017).

Foley, K. M., Roselle, S. J., Appel, K. W., Bhave, P. V., Pleim, J. E., Otte, T. L., Mathur, R., Sarwar, G., Young, J. O., Gilliam, R. C., Nolte, C. G., Kelly, J. T., Gilliland, A. B., and Bash, J. O.: Incremental testing of the Community Multiscale Air Quality (CMAQ) modeling system version 4.7, *Geosci. Model Dev.*, 3, 205–226, doi:10.5194/gmd-3-205-2010 (2010).

Guenther, A., Karl, T., Harley, P., Wiedinmyer, C., Palmer, P. I., and Geron, C.: Estimates of global terrestrial isoprene emissions using MEGAN (Model of Emissions of Gases and Aerosols from Nature), Atmos. Chem. Phys., 6, 3181-3210, https://doi.org/10.5194/acp-6-3181-2006, 2006.

Guevara, M., Martínez, F., Arévalo, G., Gassó, S., and Baldasano, J.M. An improved system for modelling Spanish emissions: HERMESv2.0. *Atmos. Environ.*, 81, 209-221 (2013).

Guevara, M., Tena, C., Porquet, M., Jorba, O., and Pérez García-Pando, C.: HERMESv3, a stand-alone multi-scale atmospheric emission modelling framework – Part 1: global and regional module, Geosci. Model Dev., 12, 1885-1907, https://doi.org/10.5194/gmd-12-1885-2019, 2019.

Haustein, K., Pérez, C., Baldasano, J.M., Jorba, O., Basart, S., Miller, R.L., Janjic, Z., Black, T., Nickovic, S., Todd, M., and Washington, R. Atmospheric dust modeling from meso to global scales with the online NMMB/BSC-Dust model: 2. Regional experiments in North Africa. Atmos. Chem. Phys., 12, 933–2958 (2012).

Janjic, Z., Gerrity Jr., J., and Nickovic, S.: An alternative approach to nonhydrostatic modeling, *Monthly Weather Review*, 129, 1164–1178 (2001).

Janjic, Z.: A nonhydrostatic model based on a new approach, *Meteorology and Atmospheric Physics*, 82, 271–285 (2003).

Janjic, Z., Huang, H., and Lu, S.: A unified atmospheric model suitable for studying transport of mineral aerosols from meso to global scales, in: IOP Conference Series: Earth and Environmental Science, vol. 7, p. 012011, IOP Publishing, 2009.

Janjic, Z. and Gall, I.: Scientific documentation of the NCEP nonhydrostatic multiscale model on the B grid (NMMB). Part 1 Dynamics, Tech. rep., Tech. rep., NCAR/TN-489+STR, doi:http://dx.doi.org/10.5065/D6WH2MZX10.5065/D6WH2MZX, 2012.

Jorba, O., Dabdub, D., Blaszczak‐Boxe, C., Pérez, C., Janjic, Z., Baldasano, J. M., Spada, M., Badia, A., and Gonçalves, M. Potential significance of photoexcited NO2 on global air quality with the NMMB/BSC chemical transport model. *J. Geophys. Res-Atmos.*, 117(D13) (2012).

Kaiser, J. W., Heil, A., Andreae, M. O., Benedetti, A., Chubarova, N., Jones, L., Morcrette, J.-J., Razinger, M., Schultz, M. G., Suttie, M., and van der Werf, G. R.: Biomass burning emissions estimated with a global fire assimilation system based on observed fire radiative power, Biogeosciences, 9, 527–554, https://doi.org/10.5194/bg-9-527-2012, 2012

Marti, A., Folch, A., Jorba, O., and Janjic, Z. Volcanic ash modeling with the on-line NMMB/BSC-ASHv1.0 model: model description, case simulation and evaluation. *Atmos. Chem. Phys.*, 17, 4005-4030 (2017).

Pay, M. T., Piot, M., Jorba, O., Gassó, S., Gonçalves, M., Basart, S., Dabdub, D., Jiménez- Guerrero, P., and Baldasano, J.M. A Full Year Evaluation of the CALIOPE-EU Air Quality Modeling System over Europe for 2004. *Atmos. Environ.*, 44, 3322-3342 (2010).

Pay, M. T., Martínez, F., Guevara, M., and Baldasano, J. M. Air quality forecasts on a kilometer-scale grid over complex Spanish terrains. *Geosci. Model Dev.*, 7, 1979-1999 (2014).

Pérez, C., Haustein, K., Janjic, Z., Jorba, O., Huneeus, N., Baldasano, J.M., Black, T., Basart, S., Nickovic, S., Miller, R.L., Perlwitz, J., Schulz, M., and Thomson, M. Atmospheric dust modeling from meso to global scales with the online NMMB/BSC-Dust model – Part 1: Model description, annual simulations and evaluation. *Atmos. Chem. Phys.*, 11, 13001-13027 (2011).

Rappenglueck, B., Lubertino,G., Alvarez, S., Golovko, J., Czader, B., and Ackermann, L.: Radical precursors and related species from traffic as observed and modeled at an urban highway junction, J. Air Waste Manage., 63, 1270–1286, https://doi.org/10.1080/10962247.2013.822438, 2013

Sander, S. P., Golden, D., Kurylo, M., Moortgat, G., Wine, P., Ravishankara, A., Kolb, C., Molina, M., Finlayson-Pitts, B., Huie, R., et al.: Chemical kinetics and photochemical data for use in atmospheric studies evaluation number 15 (2006).

Slinn, W. G. N.: Predictions for particle deposition to vegetative canopies, *Atmos. Environ.*, 16, 1785–1794 (1982).

Sofiev, M., Vankevich, R., Ermakova, T., and Hakkarainen, J.: Global mapping of maximum emission heights and resulting vertical profiles of wildfire emissions, Atmos. Chem. Phys., 13, 7039–7052 (2013).

Spada, M., Jorba, O., Pérez García-Pando, C., Janjic, Z., and Baldasano, J. M. Modeling and evaluation of the global sea-salt aerosol distribution: sensitivity to size-resolved and sea- surface temperature dependent emission schemes. *Atmos. Chem. and Phys.*, 13, 11735- 11755 (2013).

Spada, M.: Development and evaluation of an atmospheric aerosol module implemented within the NMMB/BSC-CTM, Polytechnic University of Catalonia (Ph.D. Thesis), Barcelona, Spain (2015).

Tang, Y., M. J., Lu, S., Black, T. and, J. Z., Iredell, M., Perez, C., and O., J.: Recent status of NEMS/NMMB-AQ development, paper presented at 8th Annual CMAS Conference, U.S. Environ. Prot. Agency, Chapel Hill, N. C., 2009.

Wesely, M.: Parameterization of surface resistances to gaseous dry deposition in regional-scale numerical models, Atmos. Environ., 23, 1293 – 1304 (1989).

Yarwood, G., Rao, S., Yocke, M., and Whitten, G.: Updates to the Carbon Bond Chemical Mechanism: CB05. Final Report to the US EPA, RT-0400675 (2005).

Zhang et al. (2001)

Zhang, L., Gong, S., Padro, J., and Barrie, L.: A size-segregated particle dry deposition scheme for an atmospheric aerosol module, Atmos. Environ., 35, 549–560 (2001).