10. GEM-AQ factsheet

10.1 Assimilation and forecast system: synthesis of the main characteristics

Assimilation and forecast system	
Horizontal resolution	0.1° x 0.1° latitude/longitude spherical grid
Vertical resolution	28 vertical levels up to 10 hPa. Hybrid- sigma coordinate system. 14 levels in the bottom 5km.
Gas phase chemistry	Modified ADOM IIB mechanism
Heterogeneous chemistry	Hydrolysis of N_2O_5
Aerosol size distribution	12 size bins
Inorganic aerosols	Sulphates, Nitrates
Secondary organic aerosols	Primary BC + OC and coagulation of OC
Aqueous phase chemistry	SO_2
Dry deposition/sedimentation	Gaseous species - 'big leaf' multiple resistance model (Weswely, 1989; Zhang et al., 2002); Particles – calculation of gravitational settling velocities on-line.
Mineral dust	On-line (Marticorena and Bergametti, 1995)
Sea Salt	On-line Gong-Monahan (Gong, 2003b)
Boundary values	C-IFS
Initial values	Previous day forecast from GEM-AQ
Anthropogenic emissions	CAMS-REG-AP_3.1
Biogenic emissions	MEGAN-MACC
Pollens	Birch, olive
Assimilation module	Optimal Interpolation
Observations	NRT in-situ observations (O_3, NO_2, CO, SO_2, PM_{10}, $PM_{2.5}$) distributed by Meteo-France
Frequency of assimilation	Hourly, performed once a day for the previous day
Forecast system	
Meteorological driver	12:00 UTC operational IFS forecast for the day before. The IFS data are used as boundary conditions with nesting interval of 3 hours. The extent of the piloting is shown in Figure 1.

10.2 Forward model

The GEM-AQ is an on-line chemical weather forecasting model (Kaminski et al., 2008).

10.2.1 Model geometry

The model can be configured to simulate atmospheric processes over a broad range of scales, from the global scale down to the meso-gamma scale. An arbitrarily rotated latitude-longitude mesh focuses resolution on any part of the globe. In the vertical, GEM uses the generalised sigma vertical coordinate system. It has terrain-following sigma surfaces near the ground that transform to pressure surfaces higher in the atmosphere. The model top is set at 10 hPa.

For this phase of the project, the model is run in the limited area mode (LAM) with a resolution of 0.1° x 0.1° on a spherical coordinate system. The coordinates are the following: lower-left (17,4N / 22,1W), upper-right (58.6N/ 86.6E), and are generated internally based on lower-left corner, grid extend and the numerical equator location.
The extent of the model grid is shown in Figure 4.

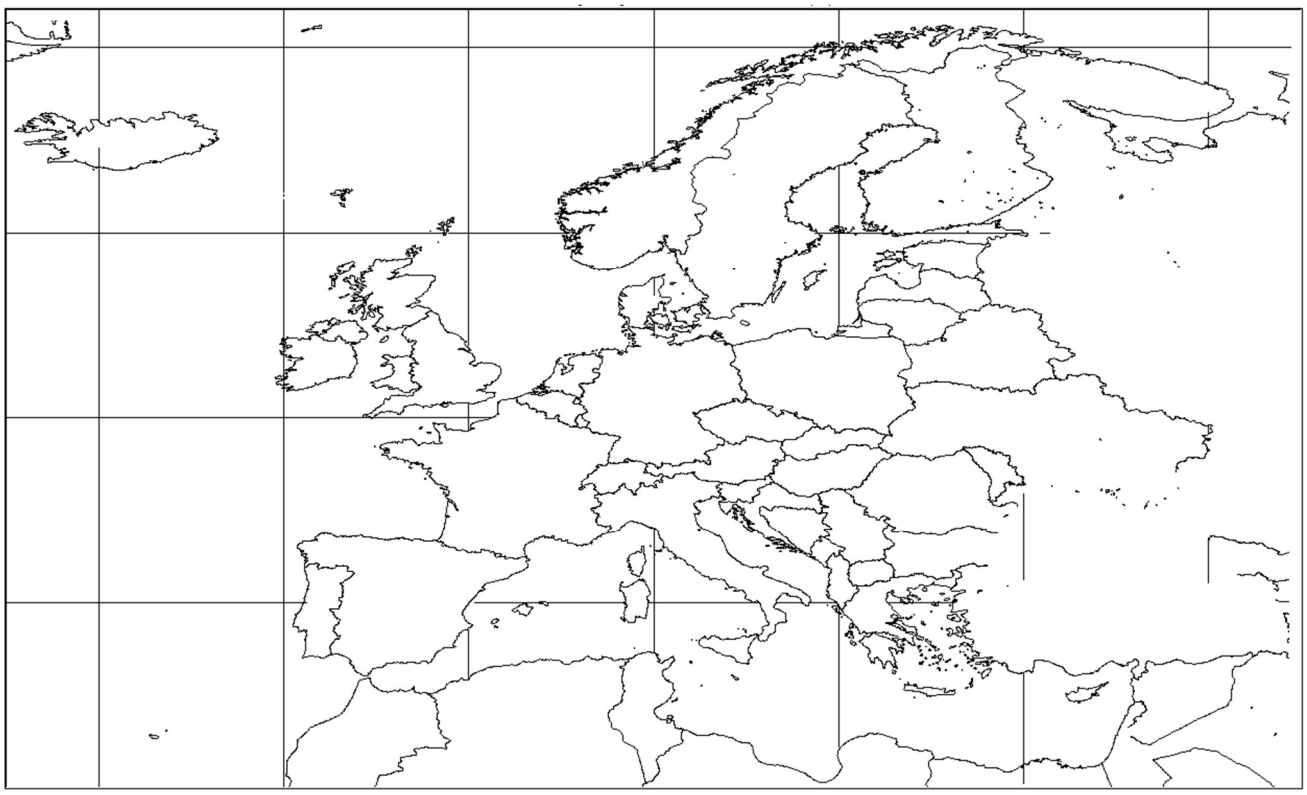

Figure 4 - GEM-AQ domain on a spherical coordinate system.

Concentrations of trace species at the fixed levels are calculated using the forecasted mixing ratio values, temperature and pressure. The surface level is represented as the first model layer. The vertical downscaling is not used to derive surface concentrations from the first model level (approximately 27 m).

10.2.2 Forcings and boundary conditions

10.2.2.1 Meteorology

The operational IFS model provides meteorological fields for initial and boundary conditions used by the GEM-AQ model. The GEM-AQ model is started using the 12-hour forecast (valid at 00 UT of the following day) as initial conditions. The IFS data are used as boundary conditions with nesting interval of 3 hours. The IFS meteorological fields are computed from spectral coefficients for the target GEM-AQ grid. Meteorological fields, within the GEM-AQ model domain, are constrained and relaxed to the IFS global model every 3 hours. Thus, the meteorological fields are 'dynamically interpolated' by the GEM meteorological model to the required transport and chemistry time steps.

10.2.2.2 Chemistry and aerosols

The C-IFS chemical fields are used as boundary conditions with nesting interval of 3 hours starting with the 24-hour forecast. The chemical and aerosol fields taken from C-IFS and used in GEM-AQ are listed in Table 10.

Table 10. The chemical and aerosol fields taken from C-IFS and used in GEM-AQ.

C-IFS Gas Phase Species	GEM-AQ Gas Phase Species
NO_2	NO_2
CO	CO
HCHO	HCHO
GO_3	O_3
NO	NO
HNO_3	HNO_3
PAN	PAN
CH_2H_6	CH_2H_6
CH_3H_8	CH_3H_8
CH_4	CH_4
SO_2	SO_2

C-IFS aerosol species	GEM-AQ aerosol species (mapping of aerosol bins in Table 11 and Table 12)
aermr04 - Dust Aerosol (0.03 - 0.55 um)	Mineral dust – distributed into 12 bins
aermr05 - Dust Aerosol (0.55 - 0.9 um)	
aermr06 - Dust Aerosol (0.9 - 20 um)	
aermr07 -Hydrophobic Organic Matter Aerosol	Organic carbon – distributed into 12 bins
aermr08 - Hydrophilic Organic Matter Aerosol	
aermr09 - Hydrophobic Black Carbon Aerosol	Black carbon – distributed into 12 bins

aermr10 - Hydrophilic Black Carbon Aerosol	
aermr11 -Sulphate Aerosol	Sulphate – distributed into 12 bins
Sea salt	Computed in the aerosol module in the GEM-AQ model

Table 11 shows mapping of C-IFS aerosol species to the GEM-AQ size bins (percentage) for mineral dust.

Table 11. Mapping of C-IFS aerosol species to the GEM-AQ size bins (percentage) for mineral dust.

GEM-AQ aerosol radius	**low**	0.005	0.01	0.02	0.04	0.08	0.16	0.32	0.64	1.28	2.56	5.12	10.24
	up	0.01	0.02	0.04	0.08	0.16	0.32	0.64	1.28	2.56	5.12	10.24	20.48
	average	0.0075	0.015	0.03	0.06	0.12	0.24	0.48	0.96	1.92	3.84	7.68	15.36
cams Dust aerosol mapping [%]		0	0	20	20	20	20	20	100	25	25	25	25
CAMS Dust Aerosol naming convention		-	-	aermr04 (0.03 - 0.55 um)					aermr05 (0.55 - 0.9 um)	aermr06 -(0.9 - 20 um)			

For organic matter aerosol, black carbon and sulphates the same log-normal based profile was applied. For organic aerosol and black carbon hydrophobic and hydrophilic components were summed as “total organic aerosol” and “total black carbon aerosol” before applying size-bin distribution profiles.

Table 12. Mapping of C-IFS aerosol species to the GEM-AQ size bins (percentage) for organic aerosol, black carbon and sulphates.

GEM-AQ aerosol radius	**lower**	0.005	0.01	0.02	0.04	0.08	0.16	0.32	0.64	1.28	2.56	5.12	10.24
	upper	0.01	0.02	0.04	0.08	0.16	0.32	0.64	1.28	2.56	5.12	10.24	20.48
	average	0.0075	0.015	0.03	0.06	0.12	0.24	0.48	0.96	1.92	3.84	7.68	15.36
Organic Mater = aermr07 + aermr08		8.0	12.3	16.1	17.8	16.5	12.8	8.5	4.5	2.1	1.0	0.3	0.1
Black Carbon = aermr09 + aermr10		8.0	12.3	16.1	17.8	16.5	12.8	8.5	4.5	2.1	1.0	0.3	0.1
Sulphates		8.0	12.3	16.1	17.8	16.5	12.8	8.5	4.5	2.1	1.0	0.3	0.1

10.2.2.3 Surface emissions

For the requested operational set-up, the anthropogenic emissions prepared in the frame of CAMS-REG-AP_v4.2/2017were used.

Anthropogenic emissions included primary gaseous and particle pollutants for individual GNFR (standardized nomenclature for air pollutants) sectors. The following fields were used: SO_2, NOx, CO, NMVOC, NH_3, PM_{10} and $PM_{2.5}$. Based on this information, emission fluxes for 15 gaseous species (9 hydrocarbons and 6 inorganics) and 4 aerosol components (primary organic aerosol, black carbon, sulphates, nitrates) were derived. Total emission flux for each aerosol component was distributed into 12 bins in the GEM-AQ aerosol module.

Anthropogenic emissions were distributed within the 7 lowest model layers (up to 1350 m) with different injection height profiles for each of the GNFR sectors. Temporal profiles modulating annual and diurnal variation of emission fluxes for each GNFR were used. Anthropogenic emissions outside the area provided by CAMS_81 were compiled using ECLIPSE_v4 (excluding aviation emissions). We consider using CAMS-GLO-ANT, test and implement in the U4 upgrade.

For biogenic emissions, monthly averaged MEGAN-MACC dataset valid for 2010 was used in order to avoid short-term variability of reactive biogenic VOC generated on-line in the model. We consider using CAMS-GLOB-BIO with the monthly resolution and test before U4.

Surface anthropogenic and biogenic emission fluxes were applied as a bottom boundary condition in the vertical diffusion equation.

10.2.3 Dynamical core

The set of non-hydrostatic Eulerian equations (with a switch to revert to the hydrostatic primitive equations) maintains the model's dynamical validity right down to the meso-gamma scales. The time discretization of the model dynamics is fully implicit, 2 time-level (Côté et al., 1998ab). The spatial discretization for the adjustment step employs a staggered Arakawa C grid that is spatially offset by half a mesh length in the meridional direction. It is second-order accurate, whereas the interpolations for the semi-Lagrangian advection are of fourth-order accuracy, except for the trajectory estimation (Yeh et al., 2002).

10.2.4 Physical parameterisations

10.2.4.1 Turbulence and convection

Deep convective processes are handled by Kain-Fritch convection parameterisation (Kain and Fritch, 1990). The vertical diffusion of momentum, heat and tracers is a fully implicit scheme based on turbulent kinetic energy (TKE) theory.

10.2.4.2 Deposition

The effects of dry deposition are included as a flux boundary condition in the vertical diffusion equation. Dry deposition velocities are calculated from a `big leaf' multiple resistance model (Wesely, 1989; Zhang et al., 2002) with aerodynamic, quasi-laminar layer, and surface resistances acting in series. The process assumes 15 land-use types and takes snow cover into account.

10.2.5 Chemistry and aerosols

10.2.5.1 Chemistry

The gas-phase chemistry mechanism currently used in the GEM-AQ model is based on a modification of version 2 of the Acid Deposition and Oxidants Model (ADOM) Venkatram et al. (1988), derived from the condensed mechanism of Lurmann (1986). The ADOM-II mechanism comprises 47 species, 98 chemical reactions and 16 photolysis reactions. In order to account for background tropospheric chemistry, 4 species (CH_3OOH, CH_3OH, CH_3O_2, and CH_3CO_3H) and 22 reactions were added. All species are solved using a mass-conserving implicit time stepping discretization, with the solution obtained using Newton's method. Heterogeneous hydrolysis of N_2O_5 is calculated using the on-line distribution of aerosol. Although the model meteorology is calculated up to 10 hPa, the focus of the chemistry is in the troposphere where all species are transported throughout the domain. To avoid the overhead of stratospheric chemistry in this version (a combined stratospheric/tropospheric chemical scheme is currently being developed), we replaced both the ozone and NOy fields with climatology above 100 hPa after each transport time step. Ozone fields are taken from the HALOE (Halogen Occultation Experiment) climatology (e.g. Hervig et al., 1993), while NOy fields are taken from the CMAM (Canadian Middle Atmosphere Model). Photolysis rates (J values) are calculated on-line every chemical time step using the method of Landgraf and Crutzen (1998). In this method, radiative transfer calculations are done using a delta-two stream approximation for 8 spectral intervals in the UV and visible applying pre-calculated effective absorption cross sections. This method also allows for scattering by cloud droplets and for clouds to be presented over a fraction of a grid cell. The host meteorological model provides both cloud cover and water content. The J value package used was developed for MESSy (Joeckel et al., 2006) and is implemented in GEM-AQ.

10.2.5.2 Aerosol

The current version of GEM-AQ has 5 size-resolved aerosols' types, viz. sea salt, sulphate, black carbon, organic carbon and dust as well as nitrates. The microphysical processes that describe the

formation and transformation of aerosols are calculated by a sectional aerosol module (Gong et al., 2003). The particle mass is distributed into 12 logarithmically spaced bins from 0.005 to 10.24-micron radius. This size distribution leads to an additional 60 advected tracers. The following aerosol processes are accounted for in the aerosol module: nucleation, condensation, coagulation, sedimentation and dry deposition, in-cloud oxidation of SO_2, in-cloud scavenging, and below-cloud scavenging by rain and snow.

10.3 Assimilation system

Data assimilation in the GEM-AQ modelling system is done with Optimal Interpolation method (i.e. Robichaud and Ménard, 2014) and is applied to the forecast. Error statistics are computed with the Hollingsworth - Lönnberg (HL) method (Hollingsworth and Lonnberg, 1986). The HL method was originally developed for the optimum interpolation method by Rutherford (1972) and refined by Hollingsworth and Lönnberg. It estimates the correlation length and the ratio of observation to model error variances by a least-square fit of a correlation model against the sample of the spatial autocorrelation of observation-minus-model residuals.

Currently, data assimilation is done at each forecast hour for O_3, NO_2, PM_{10} and $PM_{2.5}$, using surface observations provided by Meteo-France for the day before.