

GEM-AQ Fact sheet

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1.1 Assimilation and forecast system: synthesis of the main characteristics

Discretisation	Horizontal resolution	0.1° x 0.1° lat-lon spherical grid
	Number of vertical levels	28
	Top altitude	10hPa
	Depth of lower most layer	20m
	Number of lower layers	14 below 5km
Initial & boundary conditions & meteorology	Meteorological driver	D-1 12:00 UTC IFS, 3hrly
	Boundary values	CAMS-Global IFS
	Initial values	Previous forecast
Emissions: anthropogenic	Inventory	CAMS-REG v6.1 REF2 2022
	Temporal disaggregation	CAMS-REG-TEMPO_v4.1
Emissions: natural & biogenic	In-domain soil and road dust emissions	Marticorena and Bergametti, 1995
	In-domain sea-salt emissions	Gong-Monahan (Gong, 2003b)
	Birch, Grass, Olive, Ragweed, Alder, Mugwort Pollen provided by FMI	yes
	Biogenic emissions	MEGAN-MACC climatology
	Soil NOx	none
	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)
Chemistry/ Physics	Gas phase chemistry	Modified ADOM IIB mechanism, 51 species and 120 reactions
	Heterogeneous chemistry	Hydrolysis of N2O5
	Aerosol size distribution	12 bins from 10nm to 20.5µm
	Inorganic aerosols	Gong et al., (2003)
	Secondary organic aerosols	(Jiang, 2003)
	Aqueous phase chemistry	SO2 oxidation
	Dry deposition: gases	resistance approach
	Dry deposition: aerosols	gravitational settling
Wet deposition	Below cloud scavenging for soluble gas species and aerosols	
Assimilation	Assimilation method	Optimal Interpolation
	Assimilated surface pollutants	NO2, O3, PM2.5, PM10, CO, SO2
	assimilated satellite	none
	Frequency of assimilation	Hourly

1.2 Model Overview

GEM-AQ is a numerical weather prediction model where air quality processes (gas phase and aerosols) are implemented on-line in the host meteorological model, the Global Environmental Multiscale (GEM) model, developed at Environment and Climate Change Canada (Côté et al., 1998b). The model is used for operational air quality forecasting in Poland. Additionally, it is used in a research project to investigate air quality in different environmental conditions (Struzewska and Kaminski, 2008, 2012; Struzewska et al., 2016; Struzewska et al., 2015). Application of the GEM-AQ to modelling of satellite retrieved NO₂ column was carried out by (Szymankiewicz et al., 2014) and (Kawka et al., 2021).

1.3 Model geometry

The GEM-AQ 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. The model is run in the limited area mode in the CAMS regional production 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 extent and the numerical equator location. In the vertical, GEM-AQ uses the generalised sigma vertical coordinate system. It has terrain-following sigma surfaces near the ground that transform into pressure surfaces higher in the atmosphere. The model top is set at 10 hPa.

1.4 Forcing Meteorology

The operational IFS model provides meteorological fields for initial and boundary conditions used by the meteorological part of the GEM-AQ model. The GEM-AQ model is started using the 12-hour forecast (valid at 00:00 UT of the following day) as initial conditions. The IFS data are used as boundary conditions with a 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..

1.5 Chemical initial and boundary conditions

Chemical species of the CAMS Global IFS forecast for the previous day are used with a temporal resolution of 3 hours. The three available size bins from the IFS-COMBO model for dust aerosols are distributed uniformly over the 10 corresponding bins in GEM-AQ. The same log-normal profile was applied for organic matter aerosol, black carbon and sulphates. 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.

1.6 Emissions

The common annual anthropogenic emissions CAMS-REG are implemented as explained in Section 2.6.1. The following fields are available in those emissions: SO₂, NO_x, CO, NMVOC, NH₃, PM₁₀ 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) are derived using factors provided by TNO. Total emission fluxes for each aerosol component are distributed into 12 bins in the GEM-AQ aerosol module.

Anthropogenic emissions are distributed within the 7 lowest model layers (up to 1350 m) with injection height profiles for each GNFR sectors re-mapped for the GEM-AQ levels. Temporal profiles modulating annual and diurnal variation of emission fluxes for each GNFR are used.

For biogenic emissions, a monthly averaged MEGAN-MACC (Guenther et al., 2012) dataset valid for 2010 was used in order to avoid short-term variability of reactive biogenic VOC generated on-line in the model.

1.7 Solver, advection and mixing

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 discretisation of the model dynamics is fully implicit, 2 time-level (Côté et al., 1998a; Côté et al., 1998b). The spatial discretisation 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.

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

1.8 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. Wet deposition considers cloud scavenging for soluble gas species and aerosols.

1.9 Chemistry and aerosols

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 et al., 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 (CH₃OOH, CH₃OH, CH₃O₂, and CH₃CO₃H) and 22 reactions were added. All species are solved using a mass-

conserving implicit time stepping discretisation, with the solution obtained using Newton's method. Heterogeneous hydrolysis of N₂O₅ 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), both the ozone and NO_y fields are replaced with a climatology above 100 hPa after each transport time step. Ozone fields are taken from the HALOE (Halogen Occultation Experiment) climatology (Hervig et al., 1993), while NO_y fields are taken from the CMAM (Canadian Middle Atmosphere Model). Photolysis rates (J values) are calculated on-line for 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 (Jöckel et al., 2006) and is implemented in GEM-AQ.

The current version of GEM-AQ has 5 size-resolved aerosol 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 aerosol module accounts for the following aerosol processes: nucleation, condensation, coagulation, sedimentation and dry deposition, in-cloud oxidation of SO₂, in-cloud scavenging, and below-cloud scavenging by rain and snow.

1.10 Assimilation system

Data assimilation in the GEM-AQ modelling system is done with the Optimal Interpolation method (Robichaud and Ménard, 2014) and is applied to the forecasts. Error statistics are computed with the Hollingsworth-Lönnerberg (HL) method (Hollingsworth and Lönnerberg, 1986). 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.

Data assimilation is done at each forecast hour for O₃, NO₂, SO₂, CO, PM₁₀ and PM_{2.5} using surface observations.