# 9. DEHM factsheet

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

| **Assimilation and forecast system** | |
|---|---|
| Horizontal resolution | 18 km at 60°N |
| Vertical resolution | 29 vertical layers using terrain-following σ-coordinates from the surface up to 100 hPa. Lowest layer extends from the surface to about 23 m. Approximately 12 layers within the lowest 1000 m of the atmosphere. |
| Gas phase chemistry | A modified version of the Strand and Hov (1994) scheme, including an improved description of e.g. transformations of nitrogen containing compounds |
| Heterogeneous chemistry | Rates based on $NH_3$-$HNO_3$-$NH_4NO_3$ equilibrium and $NH_3$-$H_2SO_4$-$SO_4$ rates. Oxidation of $NO_2$ by $O_3$ on aerosols |
| Aerosol size distribution | 2 size fractions: $PM_{2.5}$ and coarse fraction of $PM_{10}$ |
| Inorganic aerosols | Sulphate, Nitrate and Ammonium |
| Secondary organic aerosols | Based on a VBS approach as described in Bergström et al, 2012 ("NPAS" scheme i.e. no partitioning of POA, aging of SOA) |
| Aqueous phase chemistry | $SO_2$ oxidation by $O_3$ and $H_2O_2$ (Jonson et., 2000) |
| Dry deposition/sedimentation | Gaseous and aerosol dry-deposition velocities are calculated based on the resistance method |
| Mineral dust | Apart from anthropogenic dust, also natural dust is read in at the lateral boundaries (from C-IFS) and transported within the domain |
| Sea Salt | In 2 size bins |
| Boundary values | C-IFS forecasts (global CAMS product) |
| Initial values | Previous forecast |
| Anthropogenic emissions | CAMS-REG-AP_v4_2/2017 |
| Biogenic emissions | Isoprene and monoterpenes |
| Wild fire emissions | Provided hourly GFAS emissions are included. In the forecast the latest downloaded emission for the specific hour is used. Set to zero, when more than 2 days old. |
| Forecast system | |
| Meteorological driver | 12:00 UTC operational IFS forecast for the day before |
| Assimilation system | |
| Assimilation method | New development in U3: 3D-var |

| | |
|---|---|
| In-situ observations | of $O_3$, $NO_2$, $SO_2$, CO, $PM_{2.5}$, and $PM_{10}$ – following the new station list provide in October 2020 (all stations). |
| Frequency of assimilation | At every full hour during 8:00-19:00 UTC |
| Satellite observations | None |
| Meteorological driver | operational IFS forecast and analyses for the same day (0.2°, 45 levels) |

## 9.2 Forward model

The Danish Eulerian Hemispheric Model (DEHM) is a 3-dimensional, offline, large-scale, Eulerian, atmospheric chemistry transport model (CTM) developed to study long-range transport of air pollution in the Northern Hemisphere. DEHM was originally developed in the early 1990's in our modelling group in order to study the atmospheric transport of sulphur-dioxide and sulphate into the Arctic (Christensen, 1997; Heidam et al., 1999; Heidam et al., 2004). The model has been modified, extended and updated continuously since then. The original simple sulphur-dioxide-sulphate chemistry has been replaced by a more comprehensive chemical scheme, including 73 chemical species, 9 primary particles and 158 chemical reactions.

### 9.2.1 Model geometry

The model domain used in previous studies covers most of the Northern Hemisphere, discretized on a polar stereographic projection, and includes a 2-way nesting procedure with several nests – currently up to 3 – with higher resolution over Europe, Northern Europe and Denmark. Currently the finest resolution is 5.56 km x 5.56 km for a domain covering Denmark. The vertical discretization is defined on an irregular grid with 29 layers up to ~18 km. The thickness of the lowest layer is 15–25 m. However, the definition of both the horizontal and vertical discretization is flexible and can be changed according to the applied meteorology.
Within CAMS_50, DEHM is set up with a domain including the CAMS_50 area:  25°W to 45°E and 30°N to 72°N, with an average resolution of ca. 18 km. In the coming year we will make analysis of how we can increase the resolution in order to go towards 0.1 dg. The applied DEHM domain can be seen in Figure 1, where the standard CAMS_50 domain is indicated by the blue lines.

The first/lowest model layer in DEHM has a thickness of about 23 m. In CAMS50 we deliver the concentration for this layers as the surface concentration. So downscaling is not applied. We do, however, have an option in the model to include a downscaling based on deposition rates.

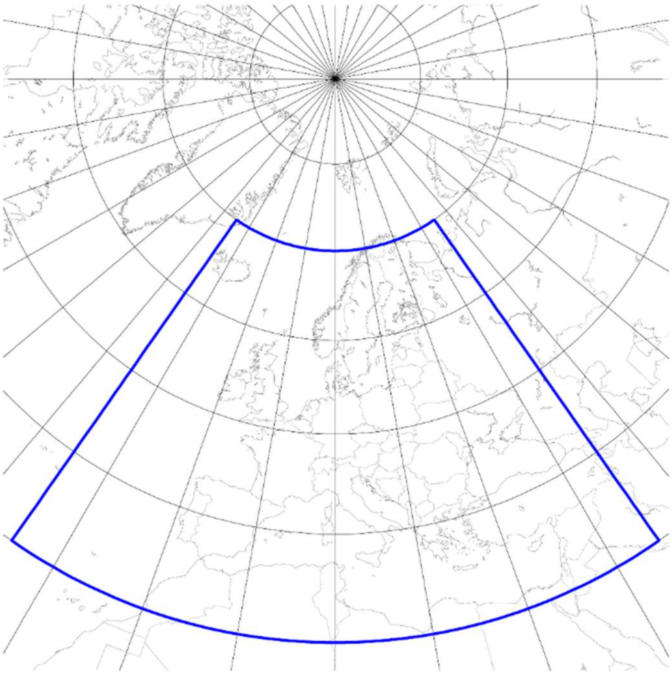

Figure 3 - The new DEHM domain and indicated by the blue lines the standard CAMS_50 domain where output is required.

### 9.2.2 Forcings and boundary conditions

#### 9.2.2.1 Meteorology

The forcing meteorology is retrieved from the IFS model system on a 0.2°x0.2° horizontal grid/45 vertical levels and with a temporal resolution of 3 hours. The meteorological data are interpolated in time and to the applied spatial grid.

#### 9.2.2.2 Chemistry and aerosols

DEHM is initialised with the C-IFS forecasts (global CAMS product) in the first initial run. Thereafter, depending on how the forecast should be set up, e.g. each daily forecast can be initialised by using the 3-d concentrations field from the DEHM-forecast at the 24-hour forecast time from the previous forecast the day before. The chemical boundary conditions for each forecast are obtained from the C-IFS forecasts starting e.g. the day before (T+24) with a 3-hour time step. The C-IFS fields included in DEHM are given in Table 1. Most of the species are linked directly to the same species in DEHM. However, it should be noted that the bins in C-IFS are not completely aligned with the 2 bins in DEHM (where fine is $PM_{2.5}$ and coarse is the non-$PM_{2.5}$ part of $PM_{10}$).

Table 9. The chemical and aerosol species taken from C-IFS and used in DEHM (updated).

| C-IFS Species | Coupled to DEHM Species |
|---|---|
| $GO_3$ | $O_3$ |
| CO | CO |
| NO | NO |
| $NO_2$ | $NO_2$ |
| PAN | PAN |
| $HNO_3$ | $HNO_3$ |
| HCHO | HCHO |
| $SO_2$ | $SO_2$ |
| $C_2H_6$ | $C_2H_6$ |
| $C_3H_8$ | goes into DEHMs group of higher alkenes |
| $C_5H_8$ | $C_5H_8$ |
| Sea Salt fine (aermr01: Sea Salt bin1 (0.03 - 0.5 um)) | Sea Salt fine |
| Sea Salt coarse (aermr02: Sea Salt bin2 (0.5 - 5 um)) | Sea Salt coarse |
| BCfresh (aermr09) | BCfresh (all in fine fraction) |
| BCaged (aermr10) | BCaged (all in fine fraction) |
| $SO_4$ (aermr11) | $SO_4$ |
| dust_aermr04 (Dust Aerosol bin 1 (0.03 - 0.55 um) | fine dust fraction |
| dust_aermr05 (Dust Aerosol bin2 (0.55 - 0.9 um) | fine dust fraction |
| dust_aermr06 Dust Aerosol bin 3 (0.9 - 20 um) | coarse dust fraction |

The link between SS and dust in the coarse and fine fraction:

SS_2.5=SS1/4.3 + 0.5 * SS2/4.3
Coarse SS = 0.5 * SS2/4.3 (as this is only the non-PM2.5 part).

Dust_2.5= dust_aermr04 + dust_aermr05
Dust_coarse= 0.4* dust_aermr06

#### 9.2.2.3 Surface emissions

The current operational version includes the CAMS-REG-AP_4.2/2017 anthropogenic emissions interpolated to the DEHM grid. Standard temporal profiles for the various SNAP sectors are applied based on profiles from the GENEMIS/EURODELTA projects (files from TNO). This includes monthly profiles pr. country, species and sector. For the daily profile, an average profile for Europe is used pr. species and sector, while an average hourly profile for Europe is used for each sector (also based on GENEMIS/EURODELTA data). Since U2 we include a matching between GNFR and SNAP following the table in GNFR_sectors_TNOemissiongrid_sept2018.pdf.

Also hourly GFAS biomass burning emissions are included. The hourly data are retrieved from the dissemination server as soon as they are available. For the forecast, we assume persistence, so that the latest downloaded emission for the specific hour is used.When the hourly emissions is more than 2 days old, it is set to zero.We also include hourly injection heights. This is calculated based on the hourly data of ‘Mean altitude of maximum injection’ and ‘Altitude of plume top’.

Natural emissions of the Biogenic Volatile Organic Compounds (BVOCs) isoprene and monoterpenes are estimated in the DEHM model based on the MEGAN model (see Zara et al. 2012 for details). The production of sea salt aerosols at the ocean surface is based on 2 parameterisation schemes describing the bubble-mediated sea spray production of smaller and larger aerosols. In each time step, the production is calculated for 10 size bins and thereafter summed up to give an aggregated production of fine (with dry diameters <1.3 um) and coarse (with dry diameters ranging 1.3-6um) aerosols (see Soares et al. 2016 for details).

### 9.2.3 Dynamical core

The horizontal advection is solved numerically using the higher order Accurate Space Derivatives scheme, documented to be very accurate (Dabdub and Seinfeld, 1994), especially when implemented in combination with a Forester filter (Forester, 1977). The vertical advection as well as the dispersion sub-models is solved using a finite elements scheme (Pepper et al., 1979) for the spatial discretization. For the temporal integration of the dispersion, the q-method (Lambert, 1991) is applied and the temporal integration of the 3 dimensional advection is carried out using a Taylor series expansion to third order. Time integration of the advection is controlled by the Courant-Friedrich-Lewy (CFL) stability criterion. An adjustment of the horizontal winds is included in order to ensure mass conservation.

### 9.2.4 Physical parameterisations

#### 9.2.4.1 Turbulence and convection

The vertical diffusion is configured by Kz profiles (Hertel et al., 1995), based on Monin-Obukhov similarity theory (see, e.g. Seinfeld, 1986) for the surface layer. This Kz profile is extended to the whole boundary layer by using a simple extrapolation, which ensures that Kz is decreasing in the upper part of the boundary layer. The planetary boundary layer (PBL) height is obtained directly from the IFS meteorology.

#### 9.2.4.2 Deposition

Gaseous and aerosol dry-deposition velocities are calculated based on the resistance method and are configured similar to the EMEP model (Simpson et al., 2003; Emberson et al., 2000), except for the dry deposition of species on water surfaces, where the deposition depends on the solubility of the chemical species and the wind speed (Hertel et al., 1995).
Wet deposition includes in-cloud and below-cloud scavenging and is calculated as the product of scavenging coefficients and the concentration of gases and particles in air. The in-cloud scavenging coefficients are dependent on Henry’s law constants and the rate at which precipitation is formed.

### 9.2.5 Chemistry and aerosols

#### 9.2.5.1 Chemistry

The basic chemical scheme in DEHM includes 74 different species and is based on the scheme by Strand and Hov (1994), but with some additions (see below). The current model describes concentration fields of 74 photo-chemical compounds (including NOx, SOx, VOC, NHx, CO, etc.). A total of 158 chemical reactions are included. Furthermore, the model has options for an additional chemical scheme for mercury (Hg) and a module for emissions and transport of persistent organic pollutants (POPs), including an extensive description of air-surface exchange of POPs for soil, water, vegetation and snow.

#### 9.2.5.2 Aerosol

The original Strand and Hov scheme has been modified in order to improve the description of, amongst other things, the transformations of nitrogen containing compounds. The chemical scheme has been extended with a detailed description of the ammonia chemistry through the inclusion of ammonia ($NH_3$) and related species: ammonium-nitrate ($NH_4NO_3$), ammonium bisulphate ($NH_4HSO_4$), ammonium sulphate ($(NH_4)_2SO_4$) and particulate nitrate ($NO_3$) formed from nitric acid ($HNO_3$) using an aerosol equilibrium approach with reaction rates dependent on the equilibrium (Frohn, 2004). Furthermore, reactions concerning the wet-phase production of particulate sulphate have been included. The photolysis rates are calculated by using a 2-stream version of the Phodis model (Kylling et al., 1995). The original rates for inorganic and organic chemistry have been updated with rates from the chemical scheme applied in the EMEP model (Simpson et al., 2003). The scheme now contains 9 classes of particulate matter ($PM_{2.5}$, $PM_{10}$, TSP, seasalt< 2.5 mm, seasalt >2.5 mm, smoke from wood stoves, fresh black carbon, aged black carbon, and organic carbon). A VBS-based approach for SOA formation has been added as part of CAMS_50 (Zare et al. 2014; Bergström et al., 2012).

## 9.3 Assimilation system

In all of CAMS50_II, we have had the development and implementation of new data assimilation scheme as one of our main development goals (as also described in the previous Developmentt reports). As part of the U3 upgrade, we have now been able to change from an optimal interpolation algorithm to a comprehensive 3D-var data assimilation scheme (Silver et al., 2016). Some of evaluation and sensitivity analysis of this is described in the latest Development Report.