MATCH Fact sheet

1.1 Assimilation and forecast system: synthesis of the main characteristics

Discretisation	Horizontal resolution	0.1° x 0.1° regular lat-lon
	Number of vertical levels	26
	Top altitude	8000m
	Depth of lower most layer	45m
	Number of lower layers	10 below 850hPa
Initial & boundary conditions & meteorology	Meteorological driver	D-1 12:00 UTC IFS, 3hrly
	Boundary values	CAMS-Global IFS
	Initial values	Previous forecast
Emissions: natural & biogenic	In-domain soil and road dust emissions	Road dust from Schaap et al. (2009) and Omstedt et al. (2005) and mineral dust based on the DEAD model of Zender et al. (2003) (mainly attributed to the Mediterranean area).
	In-domain sea-salt emissions	Sofiev et al (2011)
	Birch, Grass, Olive, Ragweed, Alder, Mugwort Pollen provided by FMI	yes
	Biogenic emissions	Simpson et al., (1995, 2012)
	Soil NOx	none
	Wildfiles emissions	Hourly emissions from D-1 for AN (D-1) and last available 24h from D-2 and D-1 cycled for FC (D+0 to D+4)
Chemistry/ Physics	Gas phase chemistry	EmChem09 (Simpson et al., 2012) and Langner et al., 1998
	Heterogeneous chemistry	Hydrolysis of N2O5, aerosol uptake of HNO3 and CH3O2H
	Aerosol size distribution	2 size fractions: PM2.5 and coarse fraction of PM10
	Inorganic aerosols	Mozurkewich, 1993
	Secondary organic aerosols	VBS schemes for ASOA and BSOA (Bergström, 2015, Bergström et al., 2012, Hodzic et al., 2016)
	Aqueous phase chemistry	SO2 oxidation
	Dry deposition: gases	resistance approach (Simpson et al., 2012)
	Dry deposition: aerosols	resistance approach (Simpson et al., 2012)
	Wet deposition	gases: species dependent in-cloud and sub-cloud scavenging ratios; particles: in-cloud scavenging ratio, sub-cloud scavenging Berge (1993) and Simpson et al. (2012)
Assimilation	Assimilation method	Intermittent 3d-var
	Assimilated surface pollutants	NO2, O3, CO, SO2, PM2.5, PM10
	assimilated satellite	
	Frequency of assimilation	Hourly

1.2 Model Overview

The Multi-scale Atmospheric Transport and Chemistry model (MATCH; Robertson et al., 1999) is an off-line chemical transport model (CTM) with a flexible design, accommodating different weather data forcing on different resolutions and projections, and a range of alternative schemes for deposition and chemistry.

1.3 Model geometry

The model geometry is taken from the input weather data. The vertical resolution is reduced with respect to the ECMWF operational model by combining pairs of IFS layers; hybrid vertical coordinates are used. The horizontal geometry of the MATCH simulation is the same as the meteorological forcing (currently a lat-lon grid with 0.1° resolution). The lowest 52 layers of the ECMWF model are used for the air quality simulations. The model top is at about 8000 m height. The model domain covers the area between 28.8° W to 45.8° E and 29.2° N to 72.0° N. The grid is an Arakawa C-grid with staggered wind components. The current operational system using various tiles of physiography derived from CCS/SEI inventory.

1.4 Forcing Meteorology

The forcing meteorology is retrieved from the 12:00 UTC run of the IFS modelling system on a 0.1°x0.1° spatial grid and with a temporal resolution of one hour. For the analyses, the 00:00 UTC analysis of the IFS is used at 0.2°x0.2° resolution. The meteorological variables included are 3D fields of the horizontal wind components (U, V), temperature, specific humidity, cloud cover, cloud water content, cloud ice water content, and surface fields of surface pressure, logarithm of surface pressure, surface temperature, sea surface temperature, snow depth, albedo, roughness height, total cloud cover, precipitation, and volumetric soil water at the surface.

1.5 Chemical initial and boundary conditions

The lateral boundary conditions for trace gases and aerosols are obtained from the IFS global forecasts at 3-hourly resolution for the following species: O_3, CO, HCHO, NO, NO_2, SO_2, HNO_3, PAN, CH_4, C_5H_8, o-xylene, sulphate and C_2H_6 (see Table 2). When the dynamic boundaries from C-IFS are missing, the model uses seasonal climatological boundary concentrations instead.

1.6 Emissions

The common annual anthropogenic emissions CAMS-REG are implemented as explained in Section 3.2. Temporal disaggregation is based on the GENEMIS tables (Ebel et al., 1997), using a GNFR to SNAP matrix. The vertical distribution of the emissions depends on the sector. Near-surface emission sources (SNAP 2,6,7,8,10) are distributed in the lowest 90 m; for other sectors the emissions are allocated over varying model levels up to a maximum of about 1100 m height. According to the sector, the anthropogenic VOC emissions are split into the MATCH chemical mechanism surrogate species: C_2H_6, NC_4H_{10}, C_2H_4, C_3H_6, OXYLENE, BENZENE, TOLUENE, CH_3OH, C_2H_5OH, HCHO, CH_3CHO, $CH_3COC_2H_5$; the particulate matter

components elemental carbon, organic matter, anthropogenic dust (other than soil and road dust) are allocated to two bins (PM2.5 and PM-coarse), as well as the road dust estimated according to Schaap et al. (2009) and Omstedt et al. (2005), and the teluric dust calculated according to Zender et al. (2003).

Biogenic emissions of isoprene, monoterpenes and sesquiterpenes are calculated following Simpson et al. (1995, 2012) and Bergström et al. (2014), taking into account temperature at 2 m, radiation fluxes and the vegetation cover. Exception is made for the isoprene oxidation for which the chain of reactions is following the Carter-1 chemical mechanism, which has proven to give the comparable results with fewer reactions (Langner et al., 1998; and Carter 1996).

The dimethyl sulphide - DMS – emissions from the Ocean and Baltic Sea are also considered; whereas the particulate matter from sea salt are calculated according to the parameterisation proposed by Sofiev et al. (2011).

The GFAS biomass burning emissions are taken into the model mapping the following species into the MATCH chemical mechanism: NOx, SO2, CO, CH4, C2H4, C2H6, C3H6, C4H10, C8H10, benzene, toluene, CH3OH, C2H5OH, formaldehyde, acetaldehyde, OC, BC, PM2.5, and PM10. The fire emissions half of these grid emissions are vertically distributed between the surface and the top of the plume (GFAS parameter) according to a parabolic curve, and the other half is uniformly distributed among the same levels.

1.7   Solver, advection and mixing

Mass conservative transport schemes are used for advection and turbulent transport. The advection is formulated as a Bott-like scheme (see Robertson et al., 1999). A second order transport scheme is used in the horizontal as well as the vertical. The vertical diffusion is described by an implicit mass conservative first order scheme, where the exchange coefficients for neutral and stable conditions are parameterized following Holtslag et al. (1991). In the convective case the turbulent Courant number is directly determined from the turnover time in the ABL.

Part of the dynamical core is the initialisation and adjustment of the horizontal wind components. This is a very important step to ensure mass conservative transport. The initialisation is based on a procedure proposed by (Heimann and Keeling, 1989), where the horizontal winds are adjusted by means of the difference between the input surface pressure tendency, and the calculated pressure tendency assumed to be an error in the divergent part of the wind field.

Boundary layer parameterisation is based on surface heat and water vapour fluxes as described by van Ulden and Holtslag (1985) for land surfaces, and Burridge and Gadd (1977) for sea surfaces. The boundary layer height is calculated from formulations proposed by Zilitinkevich and Mironov (1996) for the neutral and stable case, and from Holtslag et al. (1995) for the convective case. These parameterisations drive the formulations for dry deposition and vertical diffusion.

1.8   Deposition

Dry deposition of gases and aerosols is modelled using a resistance approach (based on the scheme in Simpson et al., 2012), which includes stomatal and non-stomatal pathways for vegetated surfaces. MATCH uses 3D-precipitation (estimated in the model, based on the surface precipitation and 3D cloud water information from the IFS forecast) and separates wet scavenging into in-cloud and sub-cloud scavenging. For most gaseous components the

scavenging is assumed to be proportional to the precipitation intensity (with higher scavenging ratios in-cloud than sub-cloud). For the particulate components in-cloud scavenging is also treated using simple scavenging ratios while the sub-cloud scavenging is treated using a scheme based on Berge (1993) with size dependent collection efficiencies (as in Simpson et al., 2012).

1.9   Chemistry and aerosols

The photochemistry scheme is based on the EMEP MSC-W chemistry scheme (Simpson et al., 2012), with a modified scheme for isoprene, based on the so-called Carter-1 mechanism (Carter, 1996; Langner et al., 1998). The SOA description is based on Hodzic et al., 2016 (Atmos. Chem. Phys. 2016, 16, 7917).

1.10   Assimilation system

The model for data assimilation is an integrated part of the MATCH modelling system. The data assimilation scheme as such is a variational spectral scheme (Kahnert, 2008), implying that the background covariance matrices are modelled in spectral space. The limitation is that covariance structures are described as isotropic and homogeneous. The advantage is that the background error matrix becomes block diagonal, and there are no scale separations as the covariance between spectral components are explicitly handled. The block diagonal elements are the covariance between wave components at model layers and chemical compounds.

Modelling the background error covariance matrices is the central part in data assimilation. This is conducted by means of the so-called NMC approach (Parish and Derber, 1992). The CTM (MATCH) is run for a 3-month period for photochemistry and aerosols with analysed and forecasted ECMWF weather data. The differences are assumed to mimic the background errors, and the statistics in spectral space are generated for different combinations of the model compounds: O3, NO2, NO, SO2, CO, PM2.5, PM10.

The scheme is fully intermittent in hour-by-hour steps and the above-listed components are assimilated from in-situ measurements. The following unobserved components are indirectly assimilated through the projection of the forecast model: NMVOCs, PAN and NH3.