SPECIAL PROJECT FINAL REPORT

Project Title:	Copernicus Atmospheric Monitoring Service – Air Quality and Composition – Regional Component (CAMS_50)
Computer Project Account:	SP DEFRIU
Start Year - End Year :	2018 - 2020
Principal Investigator(s)	Hendrik Elbern
Affiliation/Address:	Rhenish Institute for Environmental Research at the University of Cologne (RIUUK) Institute for Energy and Climate Research 8: Troposphere (IEK-8), Forschungszentrum Jülich GmbH
Other Researchers (Name/Affiliation):	Elmar Friese Institute for Energy and Climate Research 8: Troposphere (IEK-8) of the Forschungszentrum Jülich GmbH

Summary of project objectives

Copernicus Atmosphere Monitoring Service (CAMS) is establishing the core global and regional atmospheric environmental service delivered as a component of Europe's Copernicus program. The service provides continuous data and information on atmospheric composition. The service describes the current situation, forecasts the situation a few days ahead, and analyses consistently retrospective data records for recent years. CAMS has been developed to support policymakers, business and citizens with enhanced atmospheric environmental information. Formerly the Rhenish Institute for Environmental Research at the University of Cologne (RIUUK) and now the Institute for Energy and Climate Research 8: Troposphere (IEK-8) of the Forschungszentrum Jülich GmbH plays an active role in sub-project CAMS_50, which is the regional air quality component of CAMS (www.regional.atmosphere.copernicus.eu).

Summary of problems encountered

With the regular update of the CAMS_50 operational service in November 2018 the horizontal resolution of the EURAD_IM regional air quality forecast as well as air quality analysis has been increased from 15 km to 9 km. More computing time than expected at the time of application for this special project is needed for the daily model simulations with increased resolution.
Further computing time has been consumed by simulations of the impact of the COVID-19 shutdown on air quality in Europe from March to May 2020.

Experience with the Special Project framework

We are satisfied with the application procedure and with the requirements on project reporting.

Summary of results

The delivery of the European-scale air quality data within CAMS_50 is based upon a geographically distributed ensemble of currently 9 individual models under the lead of Meteo France. RIUUK provides a member of this ensemble with its comprehensive chemistry transport model EURAD-IM (Elbern et al., 2007). Three data streams are provided:

- on a daily basis, hourly analyses for the previous day and forecasts up to + 96 h;
- with a delay of a few weeks (in order to maximise the number of observations) interim re-analyses are produced daily;
- with a delay of up to 2 years (due to the delay in getting fully validated data), re-analyses are processed.

An additional important component of CAMS 50 is the further development of the individual air quality forecast models and data assimilation systems. Subject of this report are activities in the frame of CAMS_50 during the period from January 2018 to December 2020.

1. **Improvement of the EURAD-IM ozone forecast**

During the evaluation of EURAD-IM in 2016 a relatively weak performance of the ozone forecast became evident. Particularly in spring and autumn the EURAD-IM ozone forecast shows a large positive bias. In summer the peak ozone concentrations are under estimated. In order to reduce the EURAD-IM ozone forecast bias the impact of different WRF physics parameterisations on the air pollution forecast was investigated. The WRF configurations used to provide meteorological fields for the EURAD-IM forecast are summarised in Table 1. Two episodes were selected: an autumn episode from October 16 to 31, 2015 and a summer episode from July 14 to 25, 2015. The autumn episode was investigated in the second semester of 2017. It has been figured out that the meteorology computed with the current operational WRF configuration generates the largest ozone bias. The lowest bias was obtained with WRF configuration 3.

Table 1: WRF physics parameterisations

WRF configuration	Cloud Microphysics	Radiation	PBL / Surface layer	Cumulus Parameterisation
Operational	Thompson	RRTMG	MYNN	Grell-Freitas
1	Thompson	RRTMG	YSU	Grell-Freitas
2	Thompson	Dudhia	MYNN	Grell-Freitas
3	Lin (Purdue)	Dudhia	YSU	Betts-Miller-Janjic

Figure 1 shows EURAD-IM forecasts for the summer episode. The lowest maximum ozone concentrations are predicted with the current operational WRF configuration. In the simulations with WRF configuration 1 to 3 the maximum ozone concentrations are comparable and about 5 to 20 μg/m^3 higher than with the operational WRF configuration.

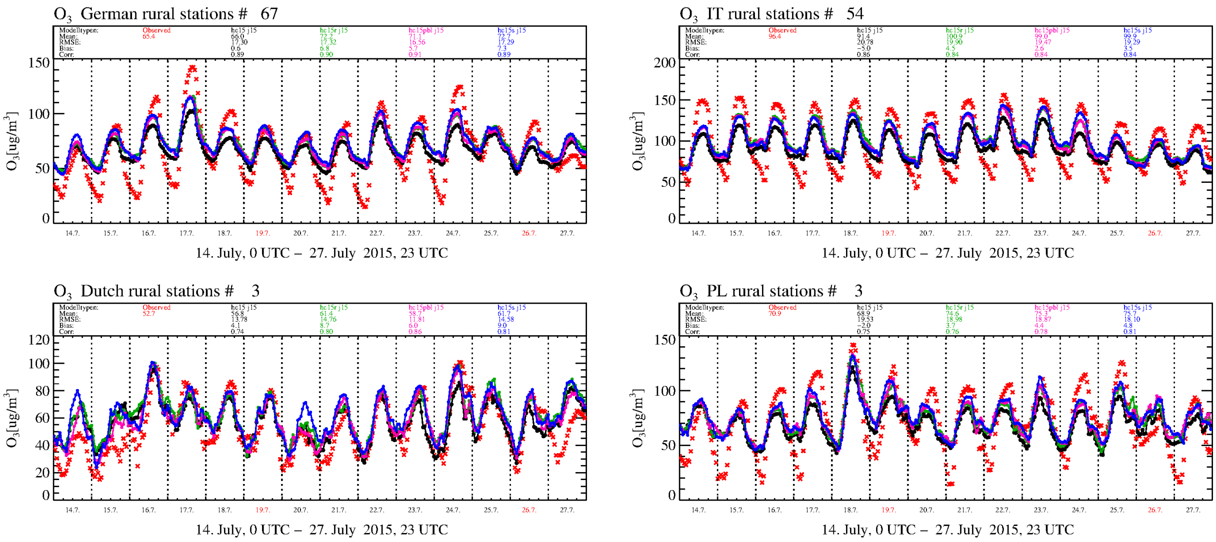


Figure 1: Ozone time-series from July 14 to 27, 2015 averaged over background surface in situ measurement sites in Germany (upper left), Italy (upper right), The Netherlands (lower left), and Poland (lower right). The EURAD-IM forecasts are based on meteorological fields computed with different WRF configurations (see Table 1). Black: current operational configuration, magenta: configuration 1, green: configuration 2, blue: configuration 3, red: measurements.

The differences between AQ forecasts with different underlying WRF meteorology are small for NO_2 and PM_{10}. From a combined evaluation of the summer and autumn episode it appears that the lowest ozone bias was obtained with WRF configuration 3. The EURAD-IM operational AQ service has been changed to this configuration at the regular update in November 2018.

2. Improvement of mineral dust module

For a mineral dust episode in April 2016 the soil texture data base used in the operational EURAD-IM configuration was replaced by the USGS soil texture data provided by WRF. The USGS data appears to be more realistic in comparison to satellite images and has a higher horizontal resolution (see Figure 2).

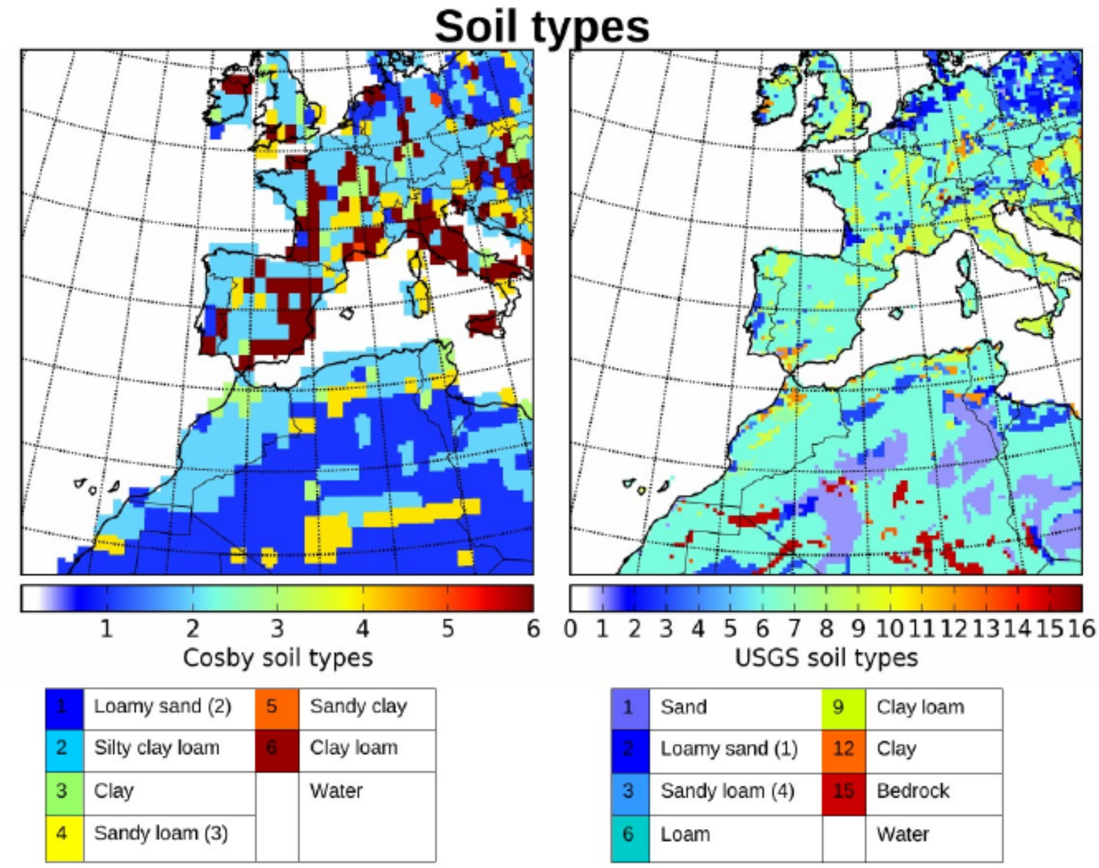
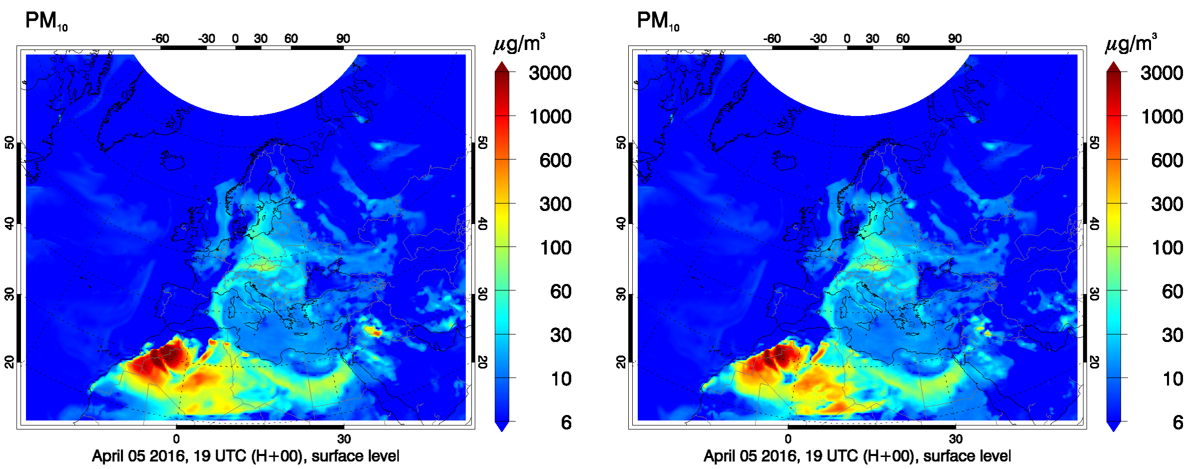


Figure 2: Soil type databases. Left: Cosby soil types used in the current operational EURAD-IM configuration, Right: USGS soil texture data provided by WRF.

A reference run in the current operational configuration of EURAD-IM and a sensitivity run using the USGS soil texture data were performed. For booth runs climatological boundary values for mineral dust were used. Mineral dust emissions were solely computed inside the model domain with DREAM (Nickovic et al., 2001). Figure 3 show a comparison of dust concentrations from the reference run and the sensitivity run for the EURAD-IM CAMS domains. PM_{10} concentrations at elevated levels are higher in the sensitivity run. A comparison of modelled PM_{10} concentrations with measurements from the EEA eReporting data base for countries with high surface PM concentrations show a very weak influence of the soil texture data on surface concentrations (see Figure 4). However, the USGS soil texture data is used since the service update in November 2018.



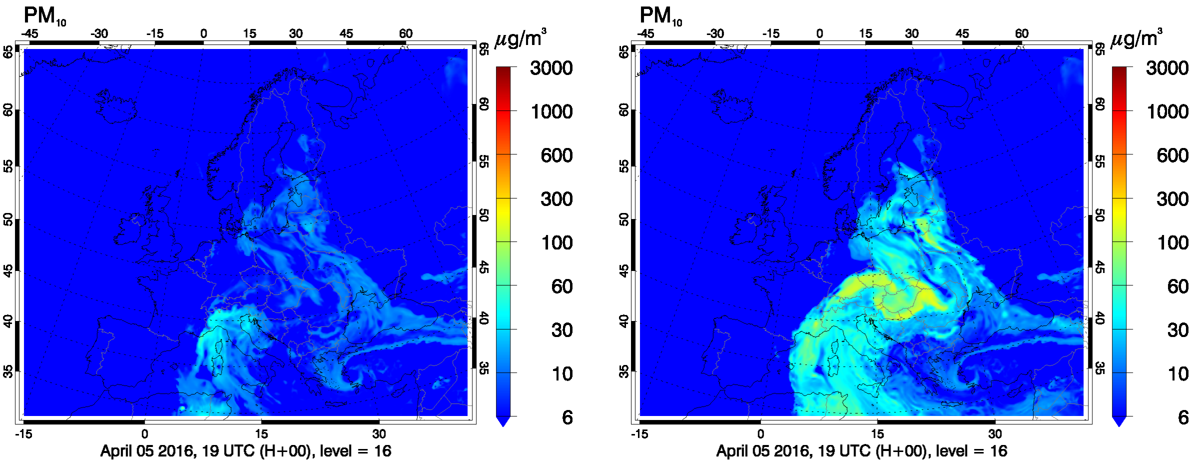


Figure 3: PM_{10} concentration for April 5, 2016 at 19:00 UTC in the near surface layer of the halo domain (above) and in level 16 of the EURAD-IM CAMS domain (below) for the reference run (left) and the sensitivity run with USGS soil texture data (right).

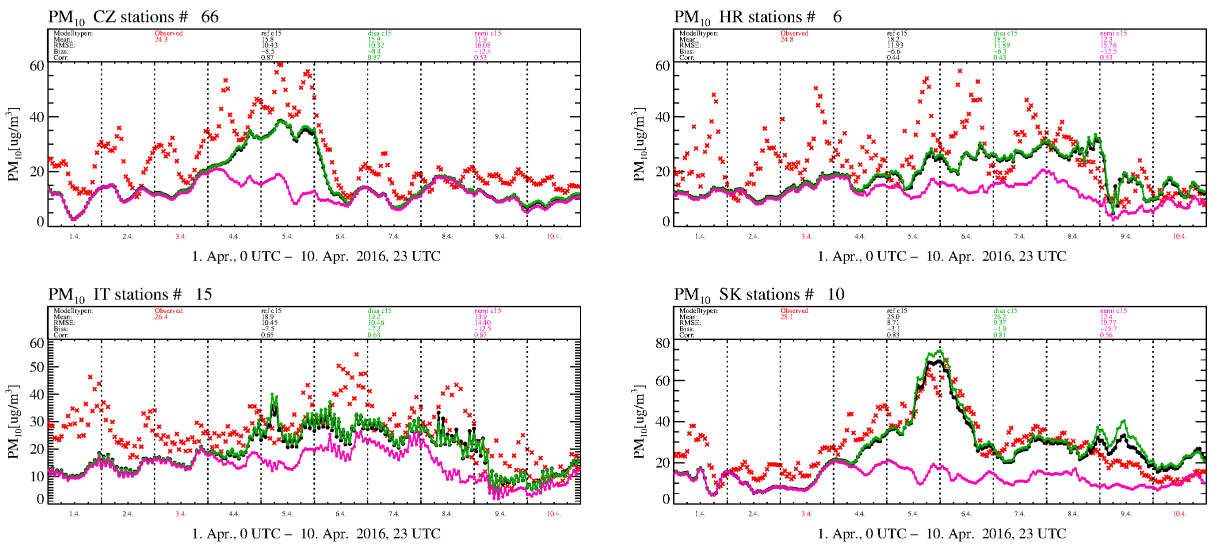


Figure 4: PM_{10} time-series from April 1 to 10, 2016 averaged over measurement sites from the EEA eReporting database for Czech Republic (upper left), Hungary (upper right), Italy (lower left), and Slovakia (lower right). Black: Reference run with EURAD-IM in current operational configuration, green: Sensitivity run with USGS soil texture data, magenta: EURAD-IM run without mineral dust emissions, red: observations.

3. Anthropogenic CAMS-REG-AP_v2.2.1 (2015) emissions

The EURAD-IM Emission Model (EEM) has been extended for the processing of emission data provided with GNFR source categories. 4 EURAD-IM simulations were set up to test this development:

- REF: A reference run with TNO MACC-III emission inventory with EEM split files (PM/VOC split, temporal profiles, injection height).
- EXP1: CAMS-REG-AP_v2.2.1 emission inventory with EEM split files.
- EXP2: CAMS-REG-AP_v2.2.1 emission inventory with CAMS-REG-AP_v2.2.1 split files.
- EXP3: CAMS-REG-AP_v2.2.1 emission inventory with CAMS-REG-AP_v2.2.1 split files and modified injection height for point sources.

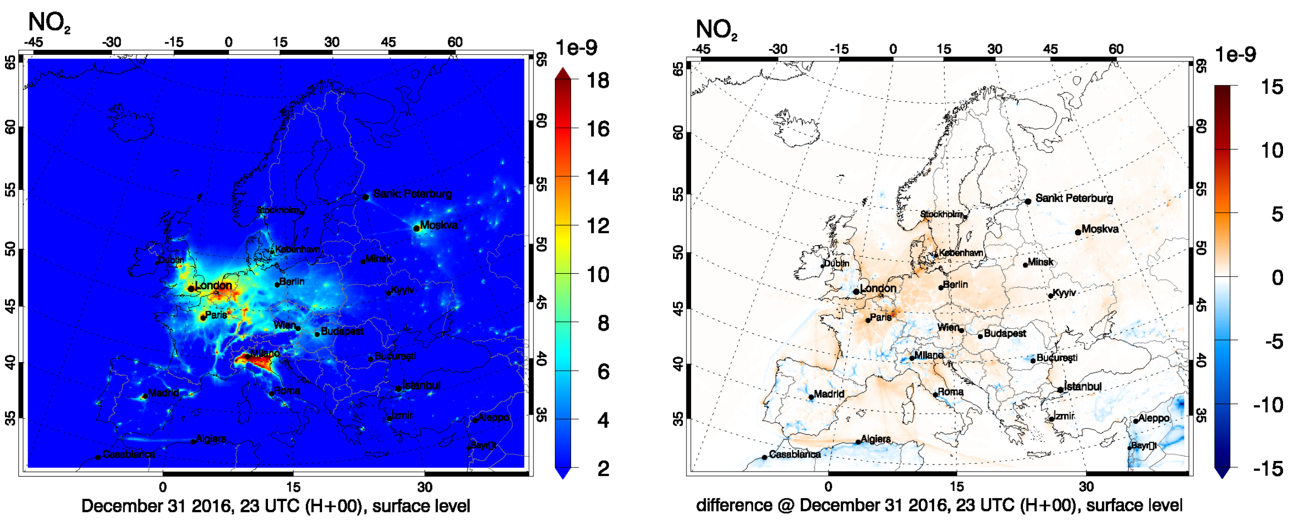
Simulation REF corresponds to the current operational EURAD-IM configuration. The model runs were conducted for August and December 2016. Figure 5 show monthly mean NO_2 concentrations for December 2016 derived from the 4 EURAD-IM simulations. Compared to the reference run (REF) the EXP1 simulation shows on average a slight increase of O_3 and a slight decrease of NO_2 and SO_2 concentrations (with the exception of North Africa and the Arabian Peninsula, which are not included in the TNO MACC-III emission inventory). PM concentrations decrease in Middle Europe and increase in Southern Europe. For CO the situation is more complex and exhibits partly a national pattern. In general, the model reflects the expectations linked to slightly decreasing emission strength between 2011 and 2015.

If the CAMS-REG-AP_v2.2.1 values for the VOC/PM split, and the temporal and vertical distribution are applied to the CAMS-REG-AP_v2.2.1 emission inventory (EXP2), O_3 concentrations generally slightly decrease and NO_2 concentrations generally slightly increase compared to the reference run. SO_2 and PM concentrations are significantly higher in EXP1 than in the reference run, especially over the Po valley and the Balkans. Again for CO the situation is more complex. In simulation EXP3 the injection heights for point sources from the GNFR sectors A (public power stations) and B (industry) were taken from the EURAD-IM emission model (EEM). In the EEM more weight is assigned to higher altitudes for point source emissions (see Table 2).

Table 2. Emission injection height for area sources and point sources

	GNFR	20m	92m	184m	324m	522m	781m	1106m
Area sources	Public power	0	0	0.25	51	45.3	3.25	0.2
	Industry	6	16	75	3	0	0	0
Point sources	Public power	0	0	0	8	46	29	17
	Industry	0	4	19	41	30	6	0

With the modified injection height the very high PM concentrations over the Balkans and the general over estimation of SO_2, which was obtained in EXP2, has been prevented. Moreover, the general positive O_3 bias and the negative bias of NO_2 and PM has been reduced compared to the reference run with TNO MACC-III emissions and compared to simulation EXP1 with CAMS-REG-AP_v2.2.1 emission inventory and EEM split files (See time-series in Figure 6). For this reason the split files used for simulation EXP3 (CAMS-REG-AP_v2.2.1 split files with modified injection height according to Table 2) have been applied in the service upgrade in June 2019.
In August 2016 the differences between the simulation experiments are small for O_3, NO_2, and CO. Again the strong over estimation of SO_2 and $PM_{2.5}$ obtained in EXP2 is not present if the injection height of point sources is modified according to Table 2. PM_{10} is still under estimated in all simulations.



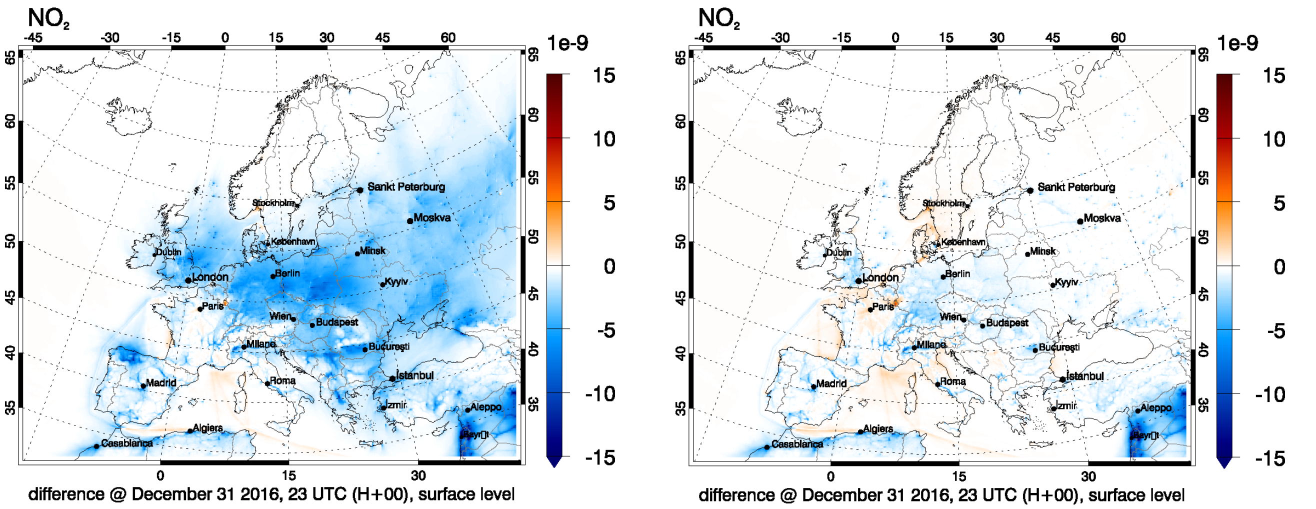


Figure 5: Monthly mean of NO_2 concentrations for December 2016 in the near surface model layer (approx. 18m). Upper left: REF simulation, upper right: difference between the simulations REF and EXP1, lower left: difference between the simulations REF and EXP2, lower right: difference between the simulations REF and EXP3. See text for explanation of the simulation identifiers.

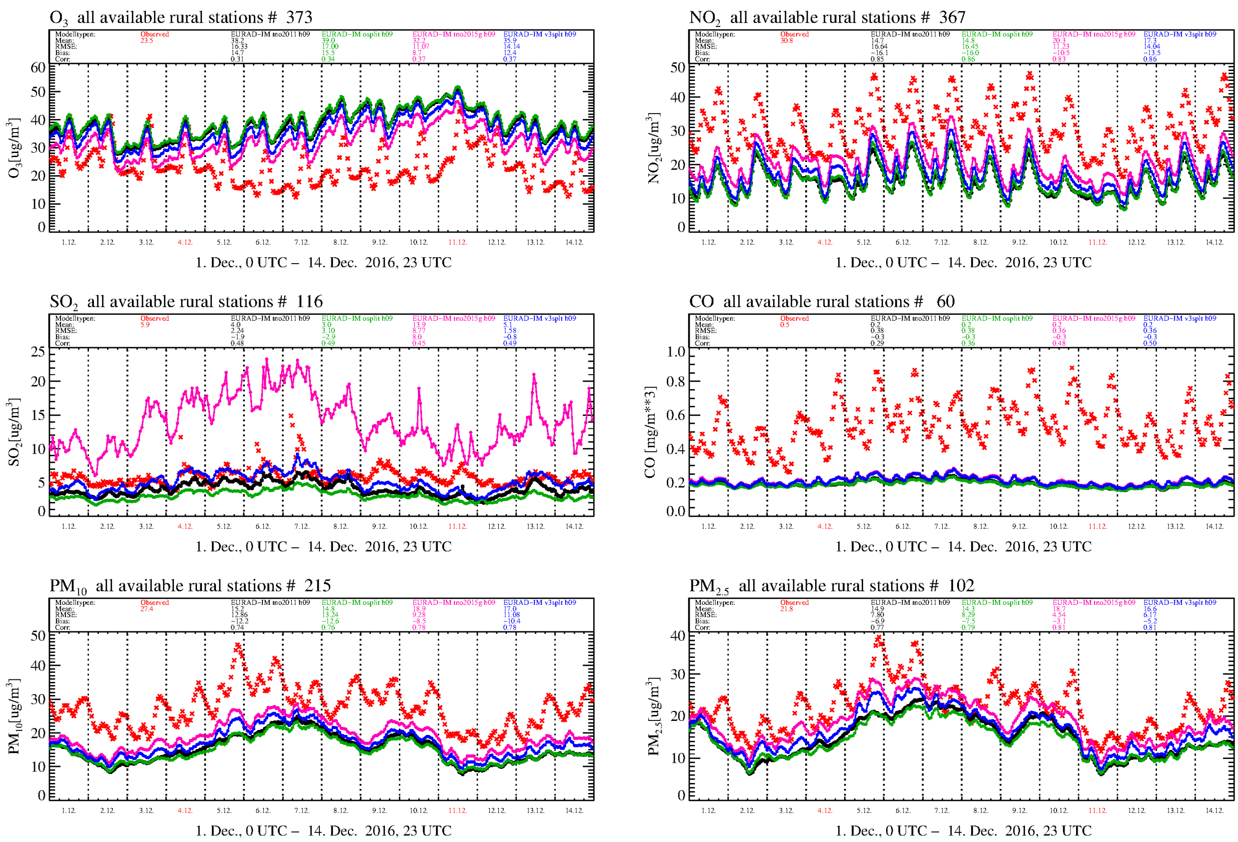
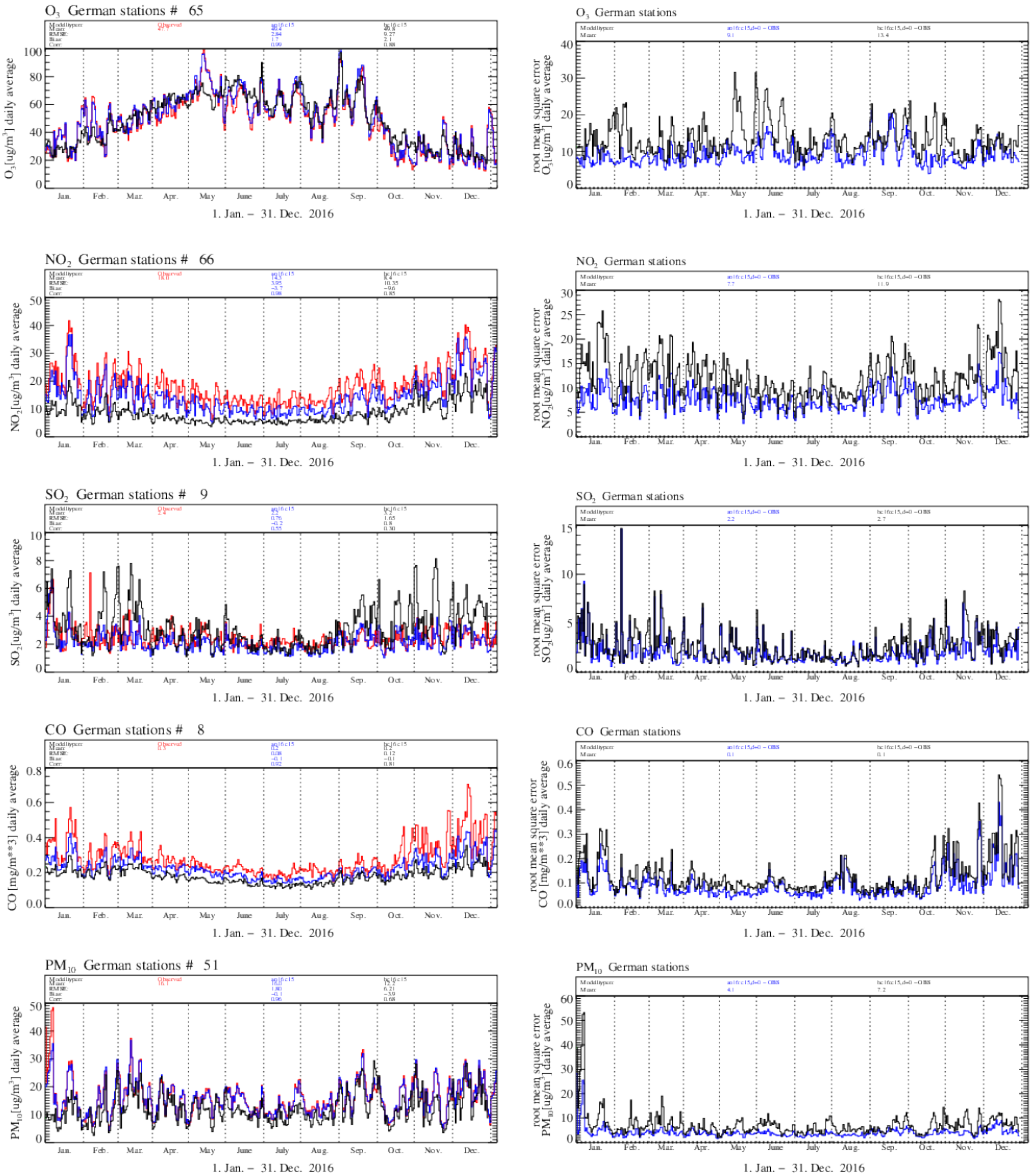


Figure 6: Time-series of O_3 (upper left), NO_2 (upper right), SO_2 (middle left), CO (middle right), PM_{10} (lower left), and $PM_{2.5}$ averaged over available EEA background surface in situ measurement sites for December 1 to 14, 2016 computed with EURAD-IM. Black: reference run (REF), Green: simulation EXP1, magenta: simulation EXP2, blue: simulation EXP3, red: observations. See text for an explanation of experiment IDs.

4. Validated assessment of air quality in Europe

An important aim of CAMS_50 is the yearly production of air quality assessment reports for

Europe. The state and the evolution of background concentrations of air pollutants in Europe are described in these reports. Validated observation and modelling data are combined in re-analysed maps and numerical fields, to propose the best available representation of air pollutant concentration fields for a spatial resolution of 0.1 deg. During the reporting period the 2016, 2017, and 2018 air quality re-analyses has been completed. The observation data assimilated consists of surface in situ data for the pollutants O_3, NO_2, SO_2, PM_{10}, and $PM_{2.5}$, the troposhperic NO_2 column content retrieved from the OMI and GOME-2 instruments, CO profile data retrieved from the MOPITT and IASI, and aircraft in situ data from IAGOS. Intermittent 3d-var data assimilation has been applied. 30% of surface in situ background stations were held back from assimilation to allow for an independent validation of the assimilation results. Figure 7 exemplary shows bias and root mean square error of daily averaged air pollutant concentrations averaged over all measurement sites, which were held back from assimilation for the year 2016.



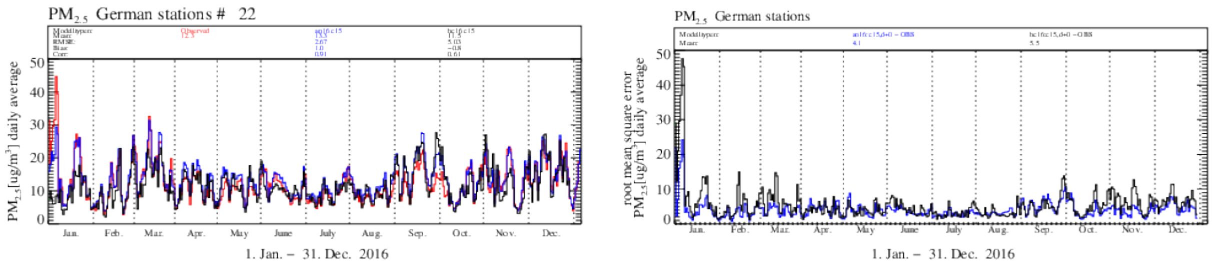


Figure 7: Daily averaged concentration (left) and its root mean square error (right) of O_3, NO_2, SO_2, CO, PM_{10}, and $PM_{2.5}$ (from above to below) averaged over all German surface in situ measurement sites, which were held back from assimilation for the year 2016. Red: observations, blue: EURAD-IM 3d-var re-analysis, 30% of stations held back from assimilation, black: control run (no data assimilation at all).

5. New aerosol species: wildfires, ECff, ECwb

2.1 Wildfire tracers

Three new aerosol species have been introduced in the EURAD-IM for the treatment of aerosols from wildfires:

PMWFi: Aitken mode aerosol from wildfires
PMWFj: Accumulation mode aerosol from wildfires
PMWFc: Coarse aerosol from wildfires

GFAS emission data is assigned to these species as follows:

$$PMWFi = 0.15 * GFAS_{2.5}$$
$$PMWFj = 0.85 * GFAS_{2.5}$$
$$PMWFc = GFAS_{tpm} – GFAS_{2.5},$$

where $GFAS_{2.5}$ is the wildfire flux of $PM_{2.5}$ (GRIB code 87.210) and $GFAS_{tpm}$ is the wildfire flux of total particulate matter (GRIB code 88.210) derived from GFAS data. The newly introduced species are considered to be chemically inert but there concentration is altered by aerosol dynamic processes treated in MADE. A tracer for aerosol with diameter lower than 10 µm from wildfires ($PMWF_{10}$) is calculated via integration over particle diameter under the assumption, that aerosols from wild fires have the same log-normal size distribution as the internally mixed aerosol species in MADE.
The development has been tested in a hindcast air quality simulation for December 2017 to February 2018. Daily GFAS data from experiment g9zk including injection height has been used for this study. $PMWF_{10}$ data has been delivered to Meteo France for validation purposes.

The former approach for the treatment of GFAS data was the following: The wildfire flux of black carbon (GRIB code 91.210) was assigned to the EURAD-IM aerosol species *anthropogenic elemental carbon (EC)*, and the wildfire flux of organic carbon (GRIB code 90.210) was assigned to the aerosol species *anthropogenic primary organic carbon (OC)*:

$$ECi = ECi + 0.15 * GFAS_{BC}$$
$$ECj = ECj + 0.85 * GFAS_{BC}$$
$$OCi = OCi + 0.15 * GFAS_{OC}$$
$$OCj = OCj + 0.85 * GFAS_{OC}$$

Aerosol species in EURAD-IM are internally mixed. Since the assignment of wildfire emissions to aerosol species has been changed, an impact on the overall PM performance is expected. Because the wildfire flux of total particulate matter was not considered in the former approach, a slight increase of the total PM concentration is expected.

2.2 ECff, ECwb

The EURAD-IM aerosol species *anthropogenic elemental carbon (EC)* has been replaced by the species *elemental carbon from fossil fuel (ECFF)* and *elemental carbon from wood burning (ECWB)*. EC emissions from GNFR sector C (other stationary combustion) are split in ECff and ECwb according to a country dependent factor provided with the CAMS-REG-AP_v3 inventory. EC emissions from other GNFR sectors are assigned to ECff. Elemental carbon emissions are distributed between the two log-normal fine aerosol modes treated in MADE as follows:

ECFFi = 0.05 * ECff
ECFFj = 0.95 * ECff
ECWBi = 0.05 * ECwb
ECWBj = 0.95 * ECwb.

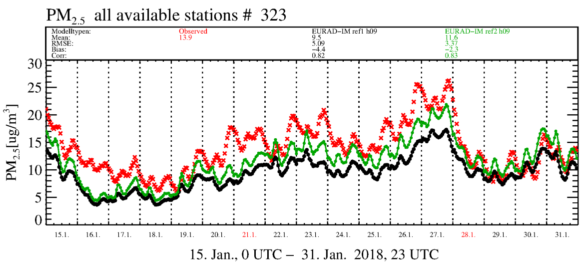
The newly introduced species are considered to be chemically inert but there concentration is altered by aerosol dynamic processes treated in MADE. Elemental carbon concentrations in the $PM_{2.5}$ fraction are calculated via integration over particle diameter under the assumption, that elemental carbon has the same log-normal size distribution as the internally mixed aerosol in MADE.
The development has been tested in a hindcast air quality simulation for December 2017 to February 2018. ECff data and ECwb data have been delivered to Meteo France for validation purposes.

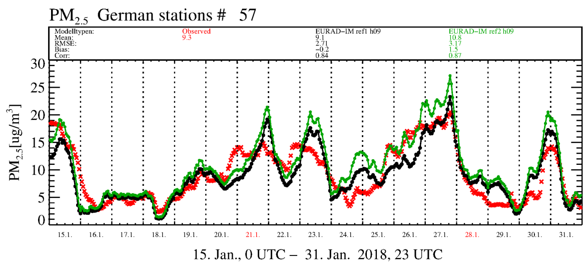
6. Voluntary contribution to the Eurodelta-Carb model intercomparison

The Eurodelta-Carb reference run (EXP A) based on CAMS-REG-AP_v4.2 emissions and a sensitivity run (EXP B) based on CAMS-REG-AP_v4.2 REF2.1 emissions including the condensable fraction in PM emissions have been performed with the EURAD-IM version developed for the treatment of elemental carbon from fossil fuel and from wood burning as described in Section 5:

A. Reference run with CAMS-REG-AP v4.2 emission data
B. Sensitivity run with CAMS-REG-AP v4.2 REF2.1 emission data and same distribution functions (vertical, temporal, PM split) as in the reference run. No assumptions have been made on volatility distribution for SVOC.

Figure 8 shows $PM_{2.5}$ time-series for the performed model runs for the period January 15 to 31, 2018. $PM_{2.5}$ concentrations in the sensitivity run are in most countries slightly to moderately higher than in the reference run. This is only a performance improvement, if $PM_{2.5}$ has a significant negative bias in the reference run. However, the overall negative $PM_{2.5}$ bias is lower, if the CAMS-REG-AP v4.2 REF2.1 emission inventory is used.





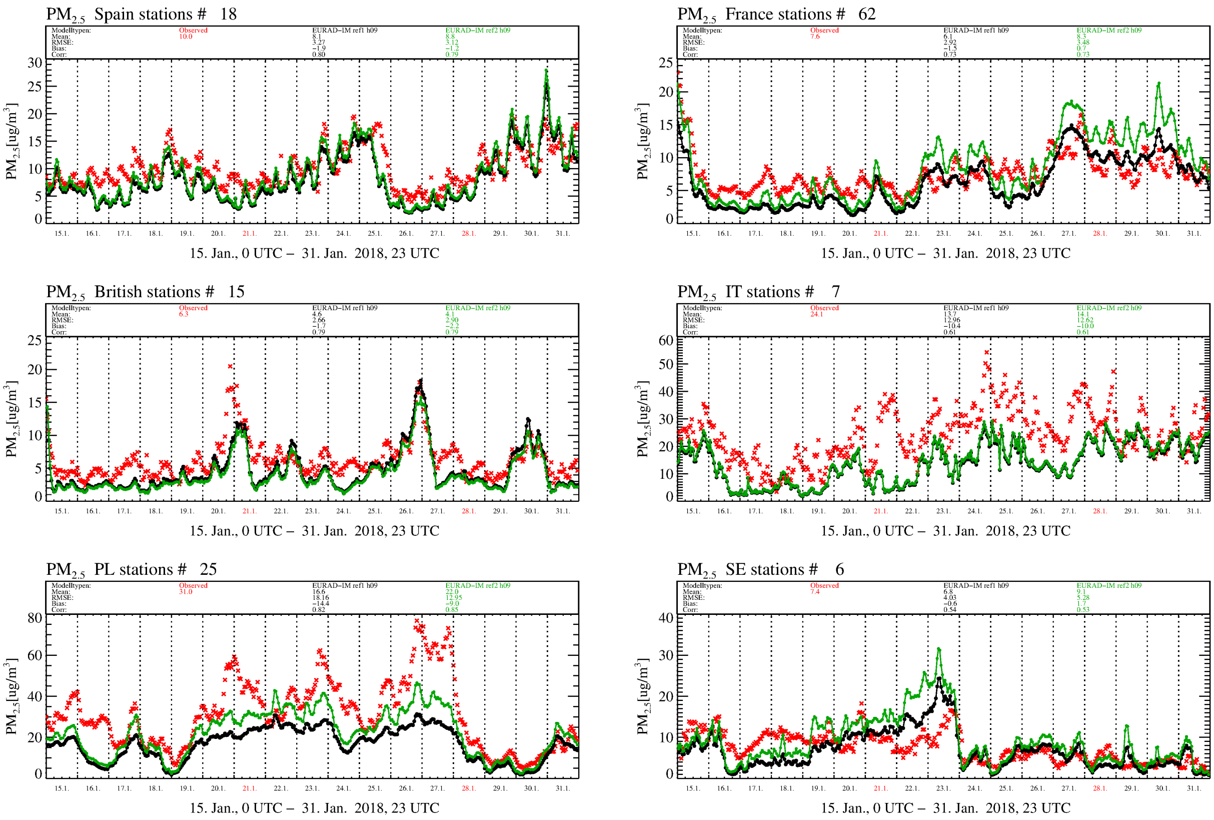


Figure 8: $PM_{2.5}$ time-series averaged over all available stations (upper left) and stations from several European countries (other panels) for January 15 to 31, 2018. Red: observations, black reference run, green: sensitivity run with CAMS-REG-AP v4.2 REF2.1 emission data.

9. Implementation of CAMS-TEMPO Temporal profiles

A set of sensitivity runs using the CAMS_TEMPO temporal emission profiles has been performed for the whole year 2018:

A. Reference run with meteorological data from the IFS analysis, chemical boundary values from the C-IFS analysis, GFAS v1.2 data, CAMS-REG-AP_v4.2 emission inventory for the year 2017, and EURAD-IM temporal emission profiles.
B. Same as the reference run with CAMS_TEMPO temporal emission profiles for the year 2018.
C. Same as the reference run with climatologic CAMS_TEMPO temporal emission profiles.
D. Same as C with a dynamic heating degree day (HDD) approach for GNFR sector C for the year 2018 provided with the CAMS_TEMPO temporal profiles.

Figures 9 exemplary show averaged times series for a northern European country (United Kingdom) and a southern European country (Spain) for a winter episode for model runs A to D.
A clear positive impact on model performance could not be obtained. Compared to the reference run peak concentrations at rush hours are higher in the sensitivity runs. PM concentrations are slightly higher for booth countries. This is also the case for SO_2 at Spanish stations. These features are an advantage only, if the model has a significant negative bias.
However, the use of gridded temporal emission profiles is an important progress, which may have the potential to improve model performance more significant in future.

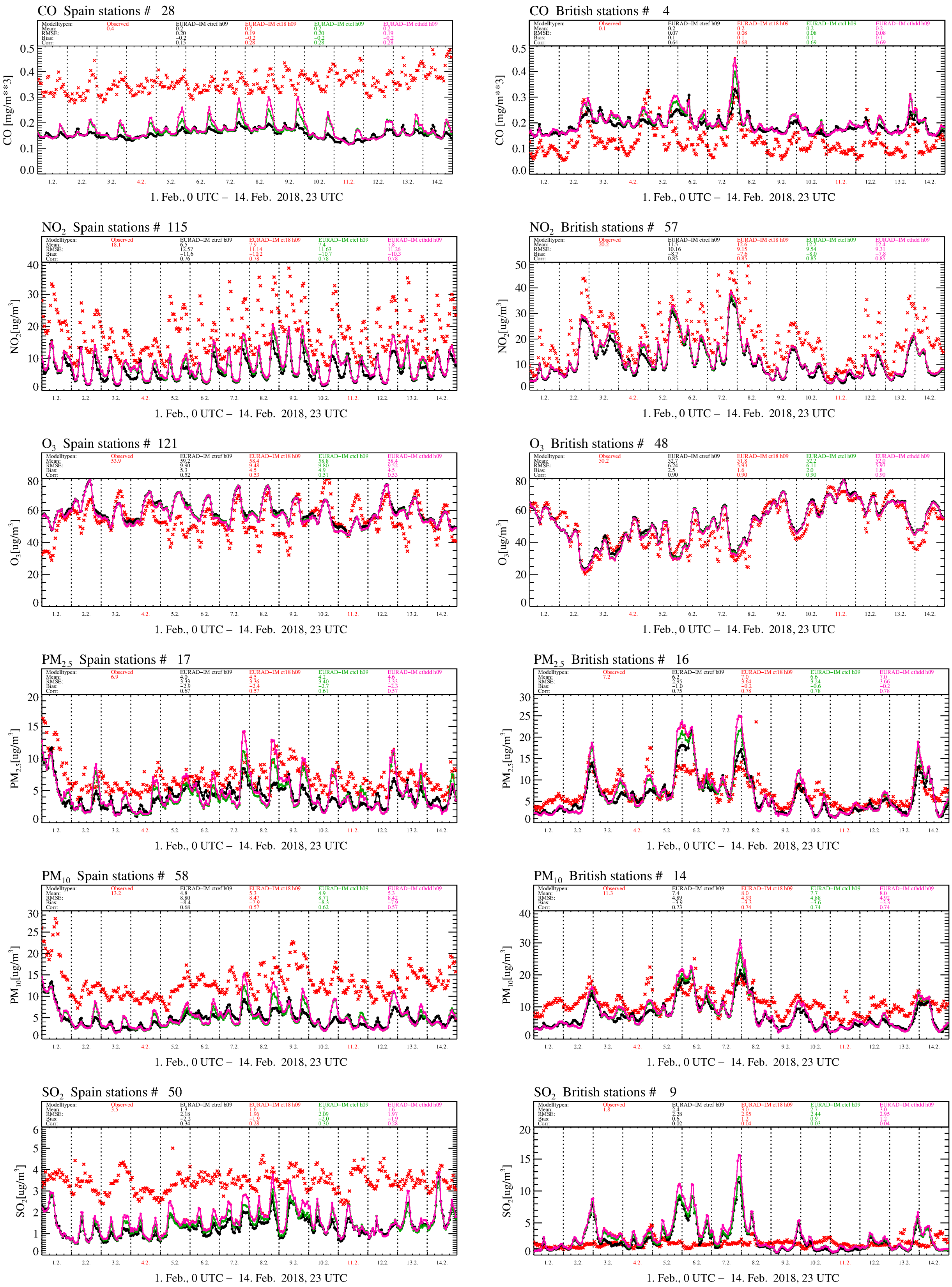


Figure 9: Time-series averaged over EEA measurement sites from Spain (left) and United Kingdom (right) for CO (above), NO_2 (second panel), O_3 (third panel), $PM_{2.5}$ (fourth panel), PM_{10}, (sixth panel), and SO_2 (below) for the period February 1 to 14, 2018. Red crosses: observations, black: reference run (run A), red: CAMS_TEMPO temporal profiles for the year 2018 (run B), green: climatologic CAMS_TEMPO temporal profiles (run C), magenta: climatologic CAMS_TEMPO temporal profiles with HDD approach for GNFR sector C (run D).

List of publications/reports from the project with complete references

Barré, J., Petetin, H., Colette, A., Guevara, M., Peuch, V.-H., Rouil, L., Engelen, R., Inness, A., Flemming, J., Pérez García-Pando, C., Bowdalo, D., Meleux, F., Geels, C., Christensen, J. H., Gauss, M., Benedictow, A., Tsyro, S., Friese, E., Struzewska, J., Kaminski, J. W., Douros, J., Timmermans, R., Robertson, L., Adani, M., Jorba, O., Joly, M., and Kouznetsov, R.: Estimating lockdown-induced European NO_2 changes using satellite and surface observations and air quality models, Atmos. Chem. Phys., 21, 7373–7394, https://doi.org/10.5194/acp-21-7373-2021, 2021.

Gama, C., Ribeiro, I, Lange, A. C., Vogel, A., Ascenso, A., Seixasa, V, Elbern, H., Borrego, C., Friese, E., Monteiro, A.: (2019). Performance assessment of CHIMERE and EURAD-IM' dust modules. Atmos. Pollut. Res., 10 (4), 1336-1347, https://doi.org/10.1016/j.apr.2019.03.005, 2019.

Future plans

The contribution of the EURAD-IM model to the Copernicus regional air quality service will probably continue within Horizon Europe project CAMS2_40.