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Urban SIS
D441.3.2 Urban air quality ECV and impact indicator data for historical conditions

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Introduction

The goal of UrbanSIS is to develop and demonstrate a method to downscale climate and impact indicators to the urban scale, delivering the information with a space/time resolution and format that makes it useful for consultants, urban planners, engineers and scientists dealing with intense rainfall, heat waves, and air pollution hazards. Within the project, WP3 targets the downscaling of climate, air quality and hydrology over three selected urban landscapes: Stockholm, Amsterdam/Rotterdam and Bologna. Simulations are carried out for historical and future time periods.

The current deliverable (D441.3.2) addresses specifically the air quality downscaling over a 5-year time window representing the historical period. Two other reports, D441.3.1 and D441.3.3, complete the work description for past conditions, respectively with the urban climate and the hydrology components. Sector-related impact indicators are included in each one of the deliverables. Future air quality data will be delivered with reports D441.3.4 to D441.3.6.

The downscaling modelling chain consists of three numerical models as depicted in Figure 1: the meteorological/climate model HARMONIE-AROME, the air quality model MATCH and the hydrological model HYPE. Emission data is provided to MATCH by Copernicus on the regional scale and by national services on the finer resolution. Essential Climate Variables (ECVs) and Sectoral Impact Indicators driven by the outputs of the models are available through the data portal.

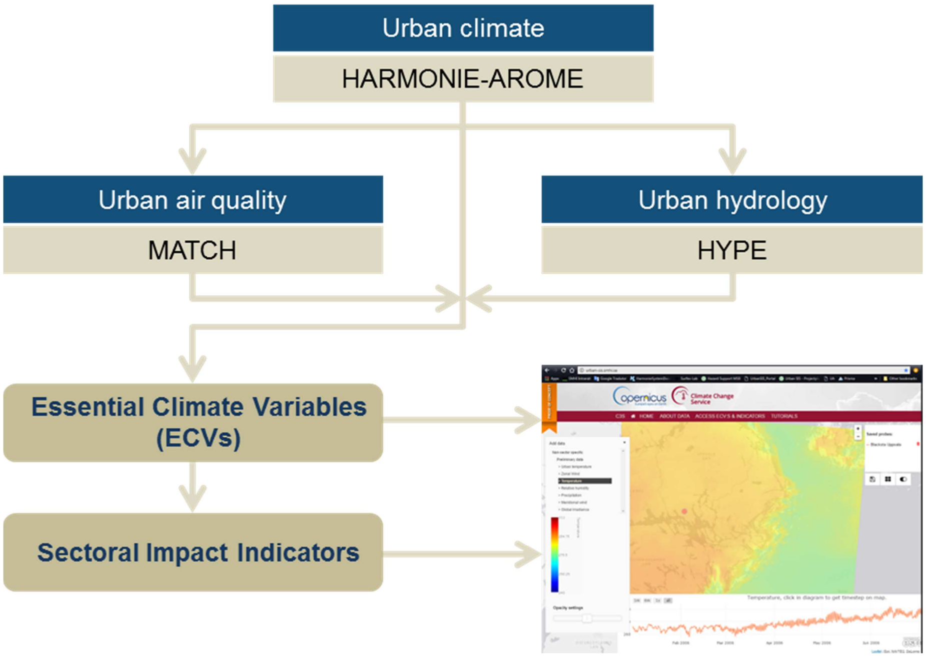

Figure 1 – General flowchart representing the downscalling approach applied in UrbanSIS. More detailed information about the air quality model MATCH will be given in the following sections.

This report summarizes relevant information about the main characteristics of the model, specific assumptions, computational domain, and input/output data. More details about the models and the numerical techniques applied can be found in the literature listed at the end of the document.

The last section of the report intends to share some experiences from the climate downscaling within UrbanSIS that can be useful for the end-users exploiting the data or for those willing to replicate this method in other European cities, in agreement with the proof-of-concept nature of this project.

1. Air quality model used for downscaling

1.1 Introduction

MATCH (Multiple-Scale Atmospheric Transport and Chemistry Modeling System) is a state-of-the-art, off-line, chemical transport model developed at the Swedish Meteorological and Hydrological Institute (SMHI). It takes three-dimensional meteorological fields from an external climate or weather forecast model and uses this meteorology to transport air pollutants with the mean wind and through turbulent mixing. The diurnal variations of physical and meteorological parameters (e.g. solar radiation, temperature, humidity) are also controlling the chemical reactions and emissions/depositions taking place at the surface-atmosphere interface. The model describes the chemistry and physical processes of an array of gaseous and particulate species. A general description of MATCH can be found in Robertson et al. (1999). The photochemical scheme is outlined in Langner et al. (1998) and Andersson et al. (2007). A recent summary and evaluation of the system's description of particulate matter can be found in Lacressonnière et al. (2017) and references therein.

In addition to meteorological forcing MATCH also needs other input data, such as temporally and spatially varying emissions and boundary concentrations of all species of interest, as shown in Figure 2. In the following sections we will focus on the various inputs to the model and touch upon some of the developments done in the present project.

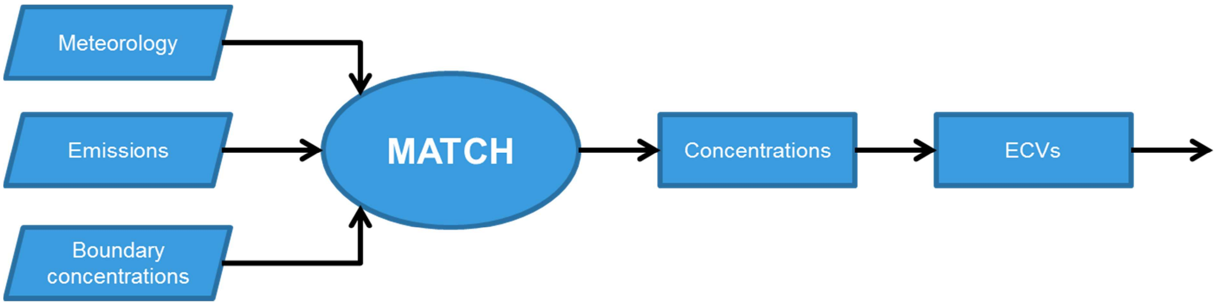

Figure 2 – Schematic structure of the data flow into and out of the off-line model MATCH.

1.2 Boundary layer parameterizations

In order to describe the surface exchange process and the vertical mixing within the boundary layer (the layer of the atmosphere closest to the ground; typically 100-2500 m in thickness, i.e. the lowest 2-15 model levels in MATCH), the time varying turbulent fluxes inside this layer must be described and quantified. The turbulence acts on scales from 100 m down to the thermal vibration of air molecules and the grid resolution does not allow for explicit description of the turbulent fluxes. Instead, we have to rely on parameterizations based on the forcing from physiography and the resolved meteorological variables (e.g. temperature, wind, humidity etc.) to derive the impact from mixing on grid cell average concentrations. Basic parameters needed to describe the turbulent mixing are listed in Table 1.

Table 1 – Boundary layer parameters.

Abbreviation	Explanation	Unit	Comment
T2m	2 m temperature	K	
Q2m	Water vapor mixing ratio	$g\ kg^{-1}$	
Ts	Surface temperature	K	Most important here is the water surface temperature
u*	Friction velocity scale	$m\ s^{-1}$	A measure of the stress the atmosphere experience from the surface
w* (*)	Turbulent velocity scale	$m\ s^{-1}$	A measure of the vertical turbulence intensity
Ri (*)	Richardson number	-	A measure of the ratio of heat and momentum gradients
F_{bv} (*)	Brunt-Vaisala frequency	s^{-1}	Wave frequency in a stable stratified layer
Zi	Boundary layer height	m	The height of the turbulent layer close to the surface: 10-2500 m
L (*)	Monin-Obukhov length	m	A measure of the stability
K_Z (*)	Vertical exchange coefficient	$m^2\ s^{-1}$	Intensity of the vertical turbulent mixing
TKE	Turbulent kinetic energy	$m^2\ s^{-2}$	A profile of turbulent intensity provided from the weather model HARMONIE–AROME

(*) Derived (i.e. calculated from other fields) variables, others are read from HARMONIE-AROME output files.

The turbulent mixing in MATCH is described by the vertical exchange coefficient, K_Z. It represents the intensity of the vertical turbulent mixing, and ranges between 1 and 150 $m^2\ s^{-1}$. The larger the value the more efficient is the turbulence to transport air pollutants vertically. In the standard MATCH configuration the variables w*, L, Zi, etc. (see Table 1) are calculated on the basis of the similarity theory. This is also the scheme used for the pan-European application of MATCH.

When using the high-resolution meteorology from HARMONIE-AROME many essential boundary layer parameters can be used directly and we therefore benefit from the boundary layer calculations made in the NWP model. The turbulent kinetic energy, TKE, is converted into K_Z by taking the square root of TKE and scale it with a length-scale defined from the Richardson number (Ri).

1.3 Precipitation

The HARMONIE-AROME model provides precipitation amounts on ground level, as well as precipitation intensities vertically on model levels. The precipitation amounts are accumulated values over the forecast length and MATCH uses this to chop up the precipitation amounts in hourly integrated values. In order to get around spin-up problems the forecasted values (that also include cloud cover and humidity) are taken from forecast length 6 to 12 hours and then jumping over the first 6 forecast hours. Attempts have been made to directly use the model level specific precipitation intensities that however did not converge to the ground precipitation amounts given in HARMONIE-AROME output. Moreover, the model level precipitation intensities are instantaneous and do not necessarily represent the integrated precipitation of the latest hour. In order to make use of the vertical precipitation information we distribute the ground precipitation vertically by means of the model level data.

2. Input to the air quality downscaling

2.1 Time period of simulation

The 5-year historical period selected is comprised of the following years: 2006, 2007, 2012, 2013, and 2014. The same period is considered for the 3 use cases. The criteria for the selection were mainly the availability of data needed by the models (namely meteorological data from UERRA and observations for assimilation and/or validation), and the project´s goal of addressing the end-user requirements and expectations. In particular, this time window responds to a specific request from Bologna end-users to consider more recent conditions, including the year 2012, which was particularly warm in the summer.

2.2 Computational domains

2.2.1 Urban air quality domain

All climate, air quality and hydrology ECVs and Sectoral Impact Indicators for each respective city are provided on a common 110×110 km^2 grid with 1 km resolution. The selection of the size, location and resolution of this area was a compromise between computational time and data amount on the one hand and the wish for as large and representative domain as possible on the other hand. 1 km × 1 km grids turned out to be a good compromise since emissions data for urban areas were generally available at this resolution. The meteorological downscalings had to be performed on a much larger area in order to be meaningful. In a too small domain the effects of local topography and land use would never have the chance to develop. Furthermore, is it advisable to exclude data close to the lateral rims of the local meteorological model as non-realistic boundary effects typically occur.

The urban air quality simulations were performed on a 120×120 km^2 grid with 1 km resolution. Figure 3 shows the extent of our three urban air quality downscaling domains together with each city’s respective 110×110 km^2 UrbanSIS area. The urban air quality simulations were performed on the geometry of the urban meteorological model but only utilizing data from a subset of its horizontal coverage. The vertical extent of the urban domain typically extended to 550 hPa (ca 5 km above surface). The vertical resolution and number of layers were reduced by a factor of two in the air quality model compared to the meteorological model by averaging all meteorological parameters over every two layers starting from the ground and extending throughout the model atmosphere.

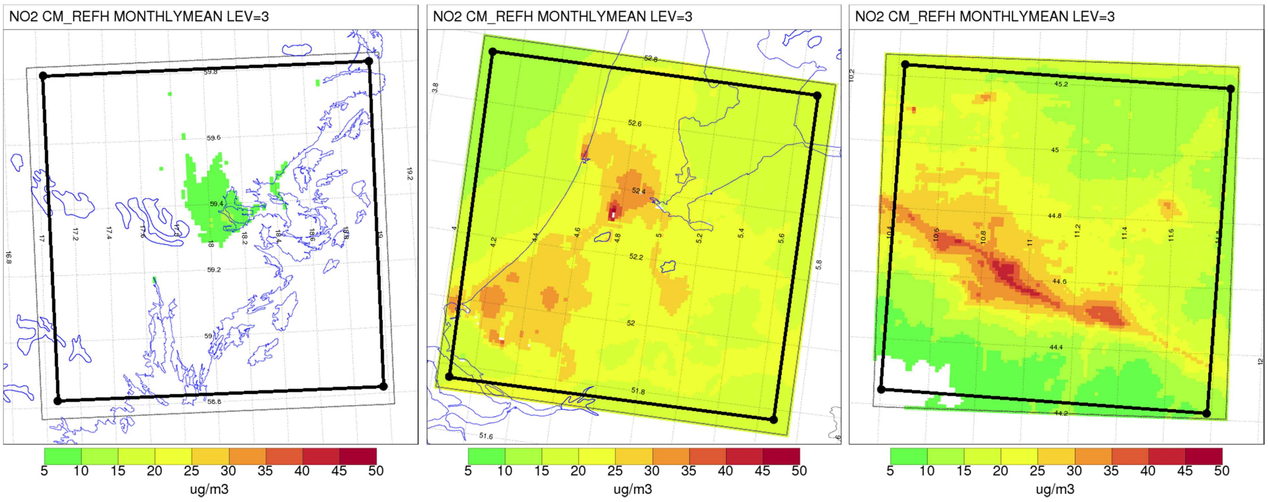

Figure 3 – Monthly mean NO_2 concentration in the three urban domains during February 2014. Left: Stockholm; Middle: Amsterdam; Right: Bologna. The extent of the 110×110 km^2 UrbanSIS areas is indicated by the fat line in the respective maps. Note the identical color scale in all panels.

2.2.2 Nesting of domains

To accurately model air quality in a city it is of utmost importance to also consider the flux of air pollutants into the domain from sources outside the city. In UrbanSIS this was achieved by running a series of nested meteorological and air quality models all simulating the same period but with varying coverage and resolution. Figure 4 outlines the principles of the nesting, which can be imagined as a series of Russian “Matryoshka” dolls where each finer domain fits into a coarser resolution outer one. An important feature is that although all set-ups run on rectangular domains they may be shifted or tilted with respect to each other due to varying geographical projections. The MATCH air quality downscaling over the urban domain covers a smaller area than the high-resolution urban meteorological model but utilizes the same geometry and resolution, which means that HARMONIE-AROME’s 1 km × 1 km meteorology is not interpolated prior to usage in the air quality model. This choice instead leads to the necessity of interpolating the local emissions and land-use data.

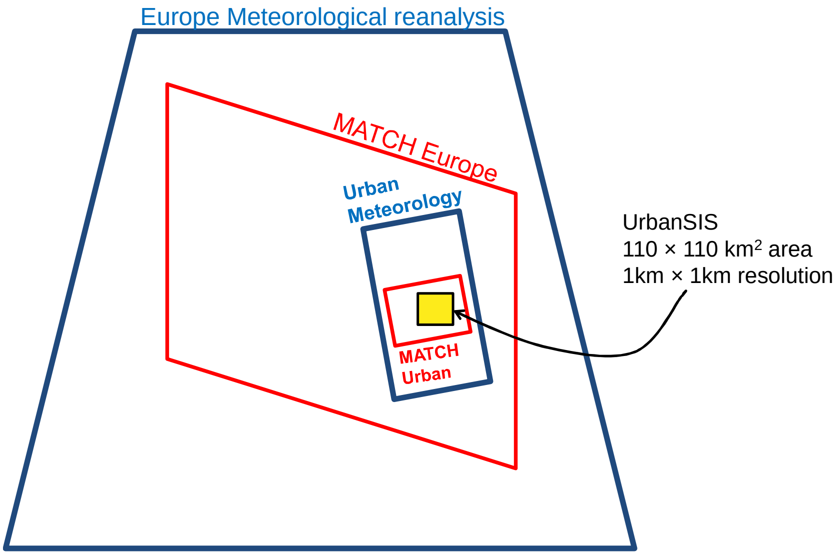

Figure 4 – Nesting of domains in UrbanSIS. The figure is not to scale. The European Meteorological reanalysis is from UERRA (Ridal et al., 2016) operating on 11 km × 11 km resolution. MATCH-Europe operates on 0.2° × 0.2° (ca. 22 km × 22 km) resolution, while the urban meteorological and air quality applications both run on 1 km × 1 km resolution.

2.3 Boundary forcing

Three-dimensional fields describing the European background and the episodic long-range transport of air pollutants were provided by first running a pan-European application of MATCH that covered Europe and adjacent regions. This set-up operated with re-analysed meteorology from UERRA (Ridal et al., 2016) and emissions data from MACC (Kuenen et al., 2014). The UERRA meteorology covers an extensive European domain on 11 km × 11 km resolution and the MACC-emissions covers a similar domain on 7 km × 7 km resolution. Computational and data-storage restrictions forced us to interpolate both the meteorology and emissions to a 0.2° × 0.2° (ca. 22 km × 22 km) resolution grid. Figure 5 shows the horizontal extent of MATCH Europe which was used for boundary concentrations for all urban downscalings. The three-dimensional boundary concentrations are interpolated horizontally and vertically to accurately describe the influx of air pollutants every 1 hour.

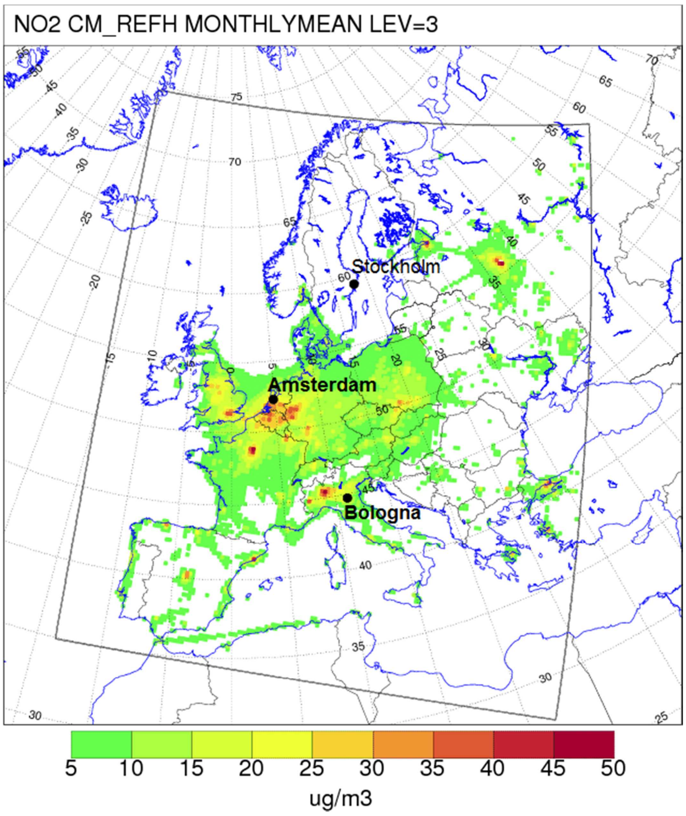

Figure 5 – Monthly mean NO_2 concentration in the European MATCH domain during February 2012. The extent of the pan-European domain and the locations of the three downscaled cities are indicated on the map.

2.4 Surface description

Embedded in the meteorological data are physiography fields which MATCH uses both for the diagnostics of the near-surface mixing and for the calculation of the deposition and emission of different chemical species. Different species have different dry deposition velocities to different surfaces and MATCH discriminates between five deposition classes (see Table 2). A number of land-types also emit biological precursors (isoprene and monoterpenes) that are important for the chemistry and physical processing of gases and particulate matter. These classes are defined in Simpson et al. (2012) and listed in Table 2 below. For the European scale MATCH simulation we use the data described in Simpson et al. (2012), while for the urban dowscalings we use the data from the AROME dataset that originates from the SURFEX package. The different tiles that come out from this are sometimes a bit exotic and different from site to site. In order to have a common ground we lump the various tiles in AROME/SURFEX to the surface and vegetation types shown in Table 2. This leads to much higher resolution in the land-cover seen by MATCH although all classes are not used.

Table 2 – List of surface types used in MATCH.

Surface type, used for BVOC emissions	Deposition class in MATCH
WATER	WATER
URBAN	URBAN
MED_BRDLF	FOREST
TEMP_DECID	FOREST
TEMP_CONIF	FOREST
MED_NDLLF	FOREST
GRASS	LOWVEG
MED_CROP	LOWVEG
WETLAND	LOWVEG
SEMI_NATURAL	LOWVEG
TUNDRA	LOWVEG
MED_SCRUB	LOWVEG
ROOT_CROP	LOWVEG
TEMP_CROP	LOWVEG
ICE_GLACIER	NOVEG
DESERT_BARREN	NOVEG

2.5 Emissions

The chain of models leading to air quality downscalings of air pollutants in different cities of Europe utilizes local emissions for the city of concern, as well as pan-European emissions used for determining the background concentrations of air pollutants. The present set-up of MATCH needs anthropogenic emissions of a number of pollutants, as listed in Table 3 below. Based on land-cover and meteorological forcing the model also performs on-line calculations of the emissions of isoprene and monoterpenes mainly important for particle formation or as precursors for ozone (O_3), cf. the discussion on the Surface description above.

In MATCH it is possible to read hourly resolved emissions or take monthly or annual two-dimensional fields which are scaled by sector-specific coefficients to mimic a typical seasonal-, weekly- and daily cycle of emissions. The sectors are the SNAP categorization (Selected Nomenclature for reporting of Air Pollutants) used by e.g. the EMEP model (see Simpson et al., 2012). In the present study we used gridded hourly data for Stockholm but annual mean data on SNAP sectors for Bologna, Amsterdam and the pan-European application. All simulated years used the same emissions data (see Table 4 below). The information about SNAP-sectors is also used to release the emissions from different sectors at different heights. The emissions from traffic and agriculture (SNAP 7 and 10) are, for example, typically released more close to surface than emissions from combustion in energy and transformation industries (SNAP 1).

Table 3 – List of anthropogenic emissions.

Species	Comment
NO_x	Split into NO and NO_2
SO_2	Split into SO_2 and sulfate
CO	
NMVOC	Split into 10 NMVOCs with different O_3 forming potential
NH_3	
PM2.5	PM less than 2.5 µm
PMcoarse	PM bigger than 2.5 µm but less than 10 µm

Table 4 – Specifics of emissions used for the different domains.

Model domain	Emission year	Type of data
Stockholm	2006	Hourly fields
Amsterdam	2013	Annual average field, 10 SNAP-sectors
Bologna	2010	Annual average field, 10 SNAP-sectors
Europe	2011	Annual average field, 10 SNAP-sectors

3. Post-processing of model output

3.1 Transformation of gridded time series to NetCDF

The gridded time series data has been converted from GRIB to netCDF format using Python and the netcdf4-python library (Unidata, https://unidata.github.io/netcdf4-python/). For each timestep the horizontal grid is re-projected into a local geographical projection (different for each city) and then a smaller grid (110x110 cells) is cut-out and stored in a netCDF file (one for each parameter).

The resulting time-series files in netCDF format have then been used as input for the calculation of ECVs and indicators.

3.2 Statistical post-processing of air quality ECVs

The statistical post-processing of air quality variables is made using the same methods and software as for the meteorological and hydrological ECVs. They have been calculated using the Climate Data Operators (CDO) software, version 1.8 (CDO 2017: Climate Data Operators, https://code.zmaw.de/projects/cdo/). For each air quality parameter, the following statistical processing is performed: mean; yearly mean; yearly max; yearly min; monthly mean; monthly max; monthly min; annual monthly mean; annual monthly max; annual monthly min; mean of yearly min; and mean of yearly max.

Note though that some combinations of parameters and statistical operators are not shown in the final results, since they are not meaningful. One such combination is yearly minimum of concentration.

3.3 Calculation of air quality indicators

Most of the indicators have been calculated using the same software as for the ECVs, the Climate Data Operators (CDO) software, version 1.8 (CDO 2017: Climate Data Operators, https://code.zmaw.de/projects/cdo/). While CDO has a large number of functions related to climate implemented, some of these differ in definition from those used in UrbanSIS, while others are not available in CDO. In such cases, the indicator has been calculated directly using Python and the netcdf4-python library (Unidata, https://unidata.github.io/netcdf4-python/), together with the NumPy library (van der Walt et al., 2011).

4. Summary of delivered air quality data

4.1 Air quality ECVs

Table 5 lists the ECVs related to air quality, defined in agreement with the requirements detailed in deliverable D4.2.

Table 5 – Summary of air quality ECVs.

ECV name	Unit
O_3 concentration	µg m^{-3}
NO_2 concentration	µg m^{-3}
PM10 concentration	µg m^{-3}
PM2.5 concentration	µg m^{-3}

As an example of an air quality related ECV, Figure 6 shows daily mean concentration of NO_2 in Bologna during 2012. San Pietro Capofiume is a rural background site outside the city while Giardini Margherita is located inside Bologna. The general level and seasonal variation with lowest concentration in summer is similar at both location, but the concentration inside the city is clearly higher than at the rural site.

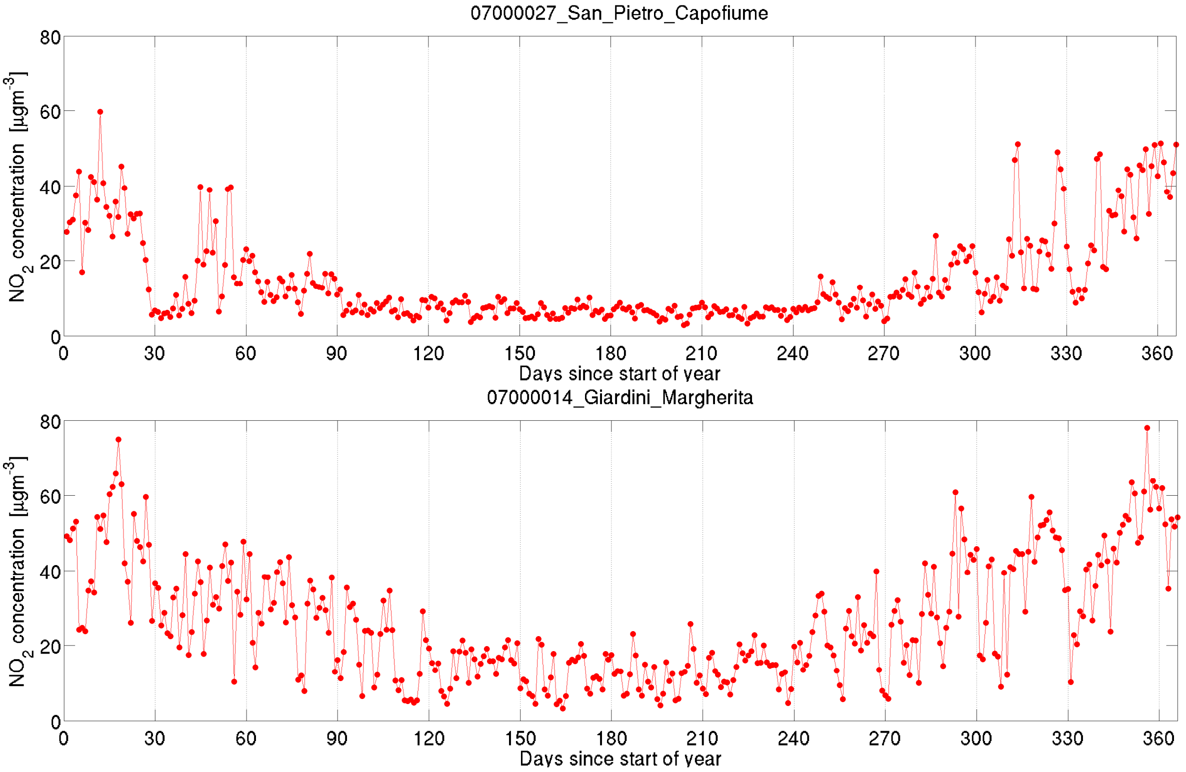

Figure 6 – Time series of daily mean NO_2 concentration at two locations in the Bologna downscaling domain during 2012.

4.2 Air quality impact indicators

Table 6 lists the indicators related to air quality. These are described in detail in report D4.3.

Table 6 – List of air quality indicators. Threshold values defined based on WHO guidelines and EU limit values. For more details see deliverable 4.3.

Sector	Type	Indicator	Aggregation	Unit	Threshold
Health	Air pollutant concentration	99.8th percentile of hourly NO_2 concentration	yearly	µg m^{-3}	200 µg m^{-3}
		Yearly average NO_2 concentration	yearly	µg m^{-3}	40 µg m^{-3}
		Yearly average PM2.5 concentrations	yearly	µg m^{-3}	25 µg m^{-3}
		Yearly average PM10 concentrations	yearly	µg m^{-3}	40 µg m^{-3}
		90th percentile of daily average PM10 concentrations	daily	µg m^{-3}	50 µg m^{-3}
		SOMO35	yearly	days µg m^{-3}	35 ppb
	Air pollution exposure	Population exposed to NO_2 conc. > AQ EU hourly limit value	yearly	persons	200 µg m^{-3}
		Population exposed to NO_2 conc. > AQ EU hourly limit value	yearly	persons	40 µg m^{-3}
		Population exposed to PM2.5 conc > AQ EU hourly limit value	yearly	persons	25 µg m^{-3}
		Population exposed to PM10 conc. > AQ EU hourly limit value	yearly	persons	40 µg m^{-3}
		Population exposed to PM10 conc. > EU daily llimit value	yearly	persons	50 µg m^{-3}
		Population exposed to O_3 conc. > EU daily target values	yearly	persons	120 µg m^{-3}
		Population exposed to O_3 conc. > WHO guidelines	yearly	persons	100 µg m^{-3}
		Population exposed to NO_2 conc. > EU hourly limit value	yearly	persons	200 µg m^{-3}
		Population exposed to NO_2 conc. > AQ EU yearly limit value	yearly	persons	40 µg m^{-3}
	Annual deaths due to NO_2 and PM2.5 long-term exposure	Mortality, all-cause, long-term NO_2 and PM2.5 exposure	yearly	deaths $year^{-1}$	
	Annual deaths due to ozone short-term exposure	Annual deaths due to O_3 short term exposure	yearly	deaths $year^{-1}$	
		Annual deaths per 100,000 inhabitants due to short term exposure	yearly	deaths 100,000 $inhab^{-1}$	

5. Experiences from the air quality downscaling

The urban air quality downscaling was the last major model simulation in a chain of model runs. Before completing these simulations it was also necessary to collate, verify and reformat an array of input data (emissions estimates and high-resolution land-use classification). Finally, we faced the challenge of reading meteorological data from HARMONIE-AROME and make use of the turbulent parameters calculated by the meteorological model, which is not the normal mode of operation of our air quality model. We clearly underestimated the extent and time requirements in all these endeavors and we did not foresee the implications in doing developments in our air quality model simultaneously as the high-resolution meteorology was being generated.

The consequence of these choices is that there is room for further developments and fine tuning of the results. Areas we know could be treated in more detail, with likely improvements in the model results include, making better use of the local information regarding the emissions (more detailed treatment of large point sources, and the utilization of local temporal profiles of the emissions, where such data exist) and fine tuning of our methods to use the high-resolution surface classification and the boundary layer parameters provided by HARMONIE-AROME.

A 1-year air quality downscaling took approximately 140 hours on 64 cores (i.e. ~9 000 CPU-hours). Ignoring the duplicate simulations performed for testing and development etc., the air quality data presented in the current report thus represents the results of 3×5×9 000 =135 000 CPU-hours of calculation on a high-performance Linux-cluster. As the air quality downscalings were so time-consuming we were forced to operate the model on a relatively small domain although we had emission data for a larger domain for most cities. Running high-resolution simulations on a high-resolution domain would probably improve the quality of the results.

A 1-year simulation on the pan-European domain, needed to provide boundary data for the urban downscalings, took ~30 hours to complete on 64 cores. The modelling domain covered an area of 172×200 cells, but as the advection time step could be kept at 300 s (instead of 20 s as in the case of the urban downscaling) these simulations were reasonably efficient. Still, there are good reasons to expect that the results would improve if we had operated the pan-European air quality model on the original resolution of the UERRA meteorology (11 km × 11 km), instead of the presently selected 22 km × 22 km (this would also increase simulation times with a factor of 4×2, as the number of grid cells would increase by a factor of 4 and the time step would need to be halved). The pan-European simulations also lacked wind-blown dust from Sahara or other arid lands. This is likely not a problem for the long-term averages but will undoubtedly result in severe underestimations of some dust episodes.

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