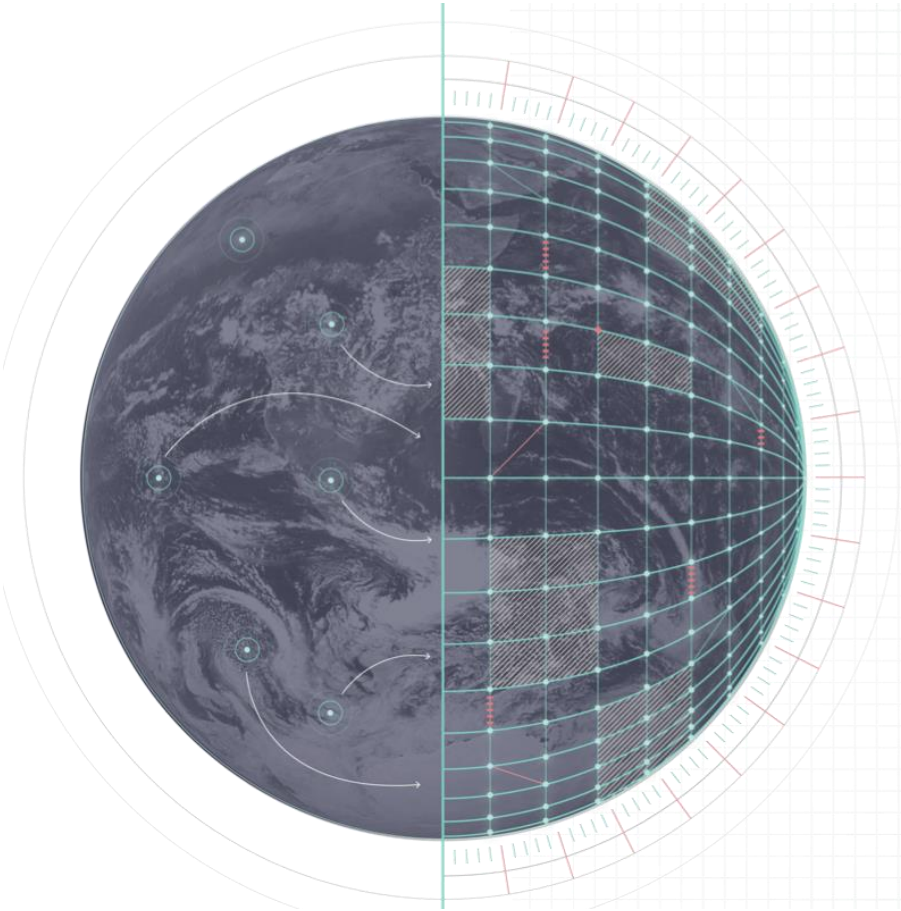


DESTINATION EARTH

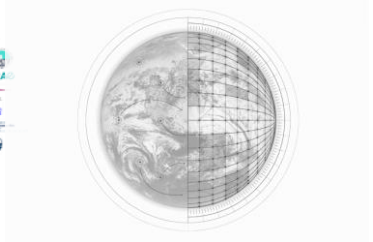
# Destination Earth On-Demand Extremes Digital Twin - **On-Demand Extremes simulations of air quality**

Marcus Hirtl
&
The On-Demand Extremes Team on the air quality impact model

2nd Destination Earth User eXchange, Bonn, Germany, 13 and 14 November 2023

Funded by the European Union

Destination Earth implemented by ECMWF esa EUMETSAT

# *DE_33070 Impact modelling – Air Quality*

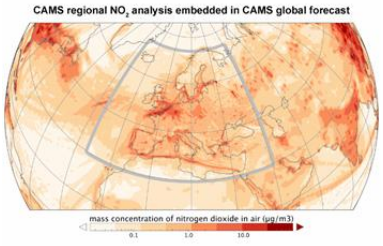
**Air pollution is a major cause of premature death and disease, and is the single largest environmental health risk in Europe.**

**Air Quality models** are important for air quality management systems:

- they are widely used by agencies tasked with controlling air pollution (e.g. predict ozone exceedances)
- identify source contributions to air quality problems
- assist in the design of effective strategies to reduce harmful air pollutants.

**Global** and **regional** modelling of air pollution ->

CAMS (global and LAM) + NMS

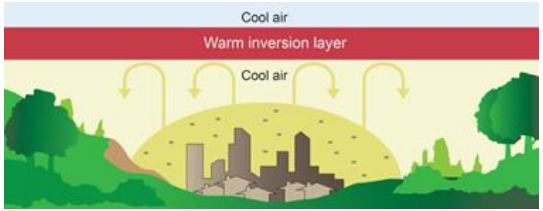


# *DE_33070 Impact modelling – Air Quality*

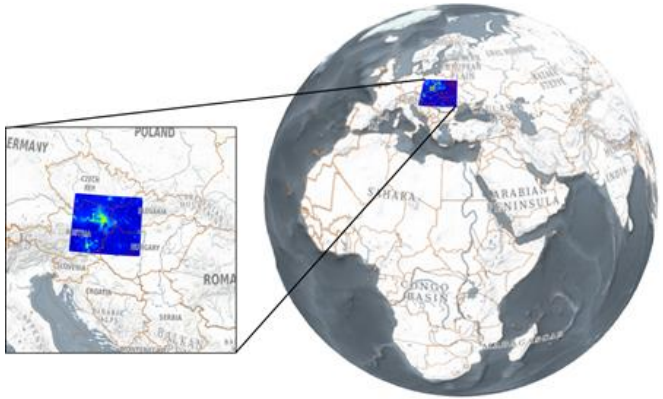
**Added value of the Air Quality model setup**

Connection between regional and city-scale. Due to very high resolution:

- Local meteorological conditions (low inversions, complex terrain)

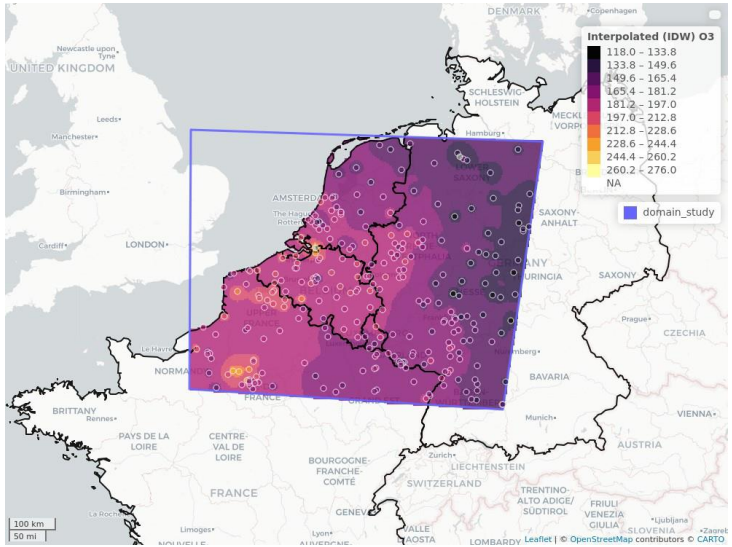



- Individual sources and source groups can be better resolved



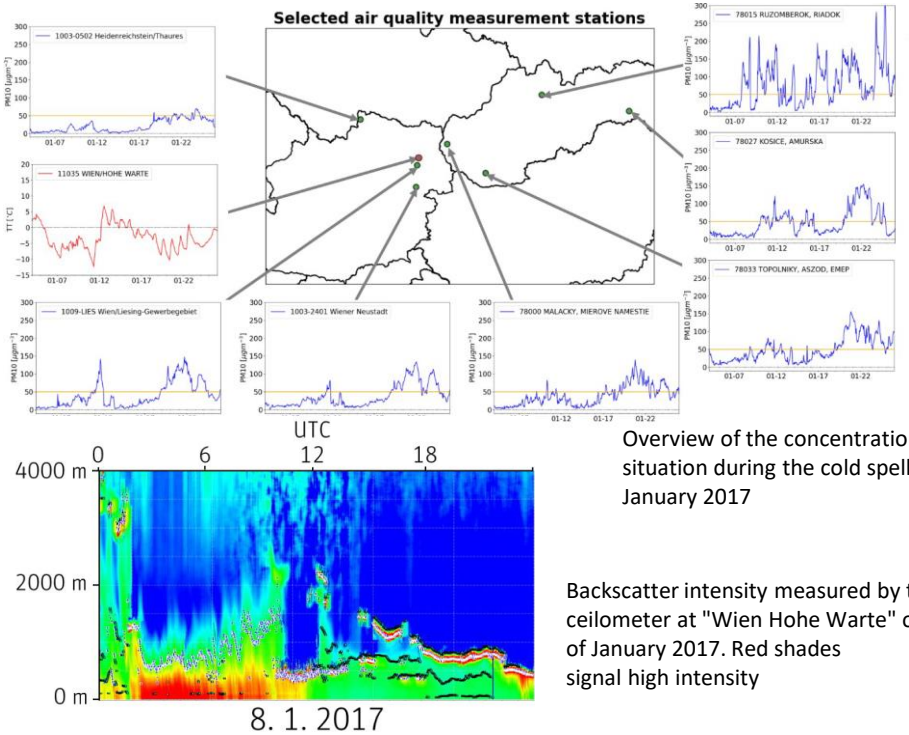
Depending on the selected use cases and domains, information on required **meteorological data** (from NWP On-Demand Extremes groups), available other input (e.g. **emissions**) and data for **model evaluation** (ground observations of pollutant concentrations), was collected.

## Summer use case 2018




Maxima of the official measurements of ozone in µg m-3 from July 24th to July 28th 2018

## Winter use case 2017




Overview of the concentration situation during the cold spells in January 2017

Backscatter intensity measured by the ceilometer at "Wien Hohe Warte" on 8th of January 2017. Red shades signal high intensity

## Extreme Digital Twin – Air Quality Impact Model

### PLANNING OUTDOOR ACTIVITIES

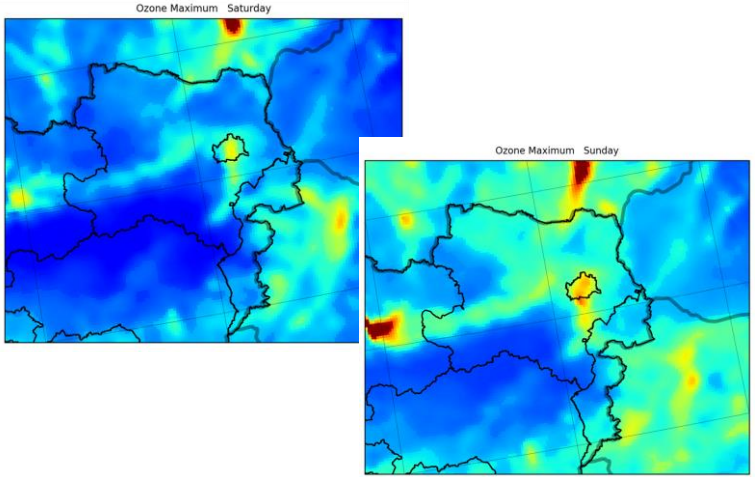
What would be a good location in vicinity of the city avoid air pollution during the weekend?

To which altitude I would have to hike up the next days to escape from the high air pollution in the valley to have a good view and healthy air?

## Extreme Digital Twin – Air Quality Impact Model

# PLANNING OUTDOOR ACTIVITIES

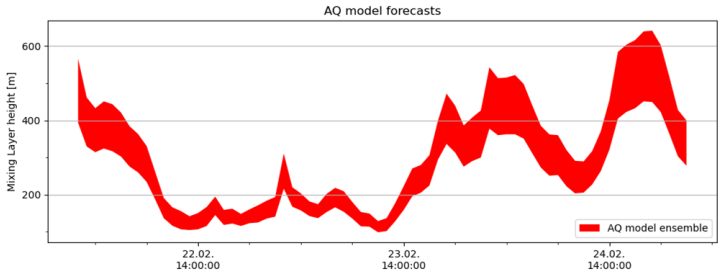
Due to the weather conditions, we expect the maximum of the ozone plume south of the city on Saturday, northern parts have much better air quality on that day, on Sunday the situation is worse in the whole region. We suggest Saturday for outdoor activities.




We advice to climb up altitudes above

- 300 m on the 22nd Feb
- 600 m on the 23rd Feb

to reach “clean air”, which lies over the inversion in the valley.



# *DE_33070 Impact modelling – Air Quality*

The emphasis of phase 1 of On-Demand Extremes is to prepare the individual AQ-models for sub 1 km resolutions, to harmonise input data and output data formats amongst models and to show the added value of the applications to stakeholders.

Task 33071: **Requirements definition**

Task 33072: **Input data collection and preparation**

Task 33073: **AQ-model setup and demonstration region**

Task 33074: **Implementation of the on-demand configurable system and application for use cases**

Task 33075: **Ensemble development**

Task 33076: **Evaluation**

| Year | Year 2022 | | | | | | Year 2023 | | | | | | | | | | | | Year 2024 | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Semester | Semester 2-2022 | | | | | | Semester 1-2023 | | | | | | Semester 2-2023 | | | | | | Semester 1-2024 | | | |
| Month | Jul | Aug | Sep | Oct | Nov | Dec | Jan | Feb | Mar | Apr | May | Jun | Jul | Aug | Sep | Oct | Nov | Dec | Jan | Feb | Mar | Apr |
| Month no. | M1 | M2 | M3 | M4 | M5 | M6 | M7 | M8 | M9 | M10 | M11 | M12 | M13 | M14 | M15 | M16 | M17 | M18 | M19 | M20 | M21 | M22 |
| WP7 Impact modelling - Air quality | | | | | | | | | | | | | | | | | | | | | | |
| Task 1 Requirements definition | | | | | | D7.1.1 M7.1.1 | | | | | | | | | | | | | | | | |
| Task 2 Input data collection and preparation | | | | | | D7.2.1 M7.2.1 M7.2.2 | | | | | | | | | | | | | | | | |
| Task 3 AQ-model setup and demonstration region | | | | | | | | | | | | D7.3.1 M.7.3.1 | | | | | | | | | | |
| Task 4 Implementation of the on-demand configurable system and application for use cases | | | | | | | | | | | | | | | | | | | | | D7.4.1 M7.4.1 | |
| Task 5 Ensemble development | | | | | | | | | | | | D7.5.1 | | | | | | | | | | |
| Task 6 Evaluation | | | | | | | | | | | | | | | | | | | | | D7.6.1 M7.6.1 | |

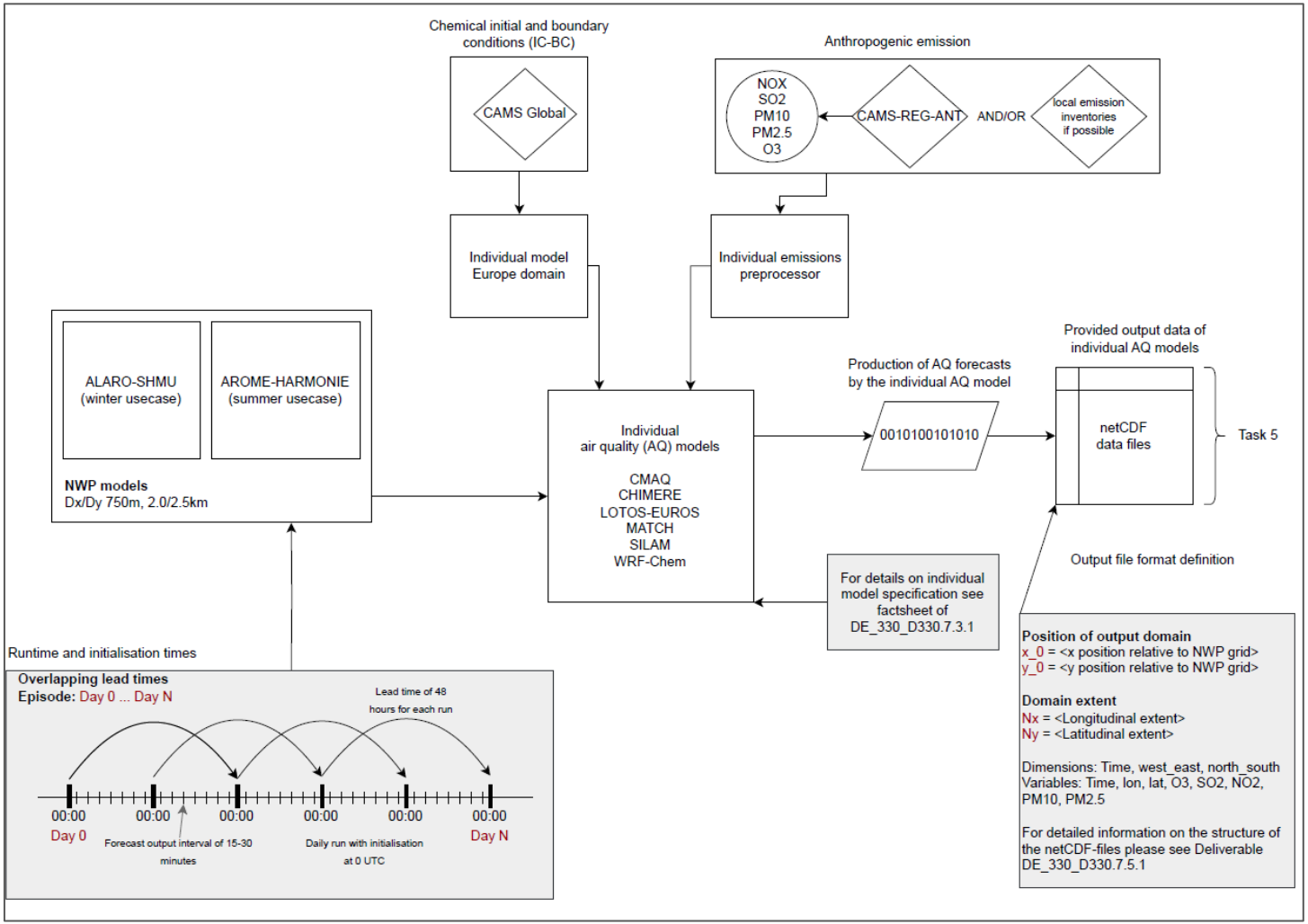
# Implementation for the on-demand configurable system and application for use cases

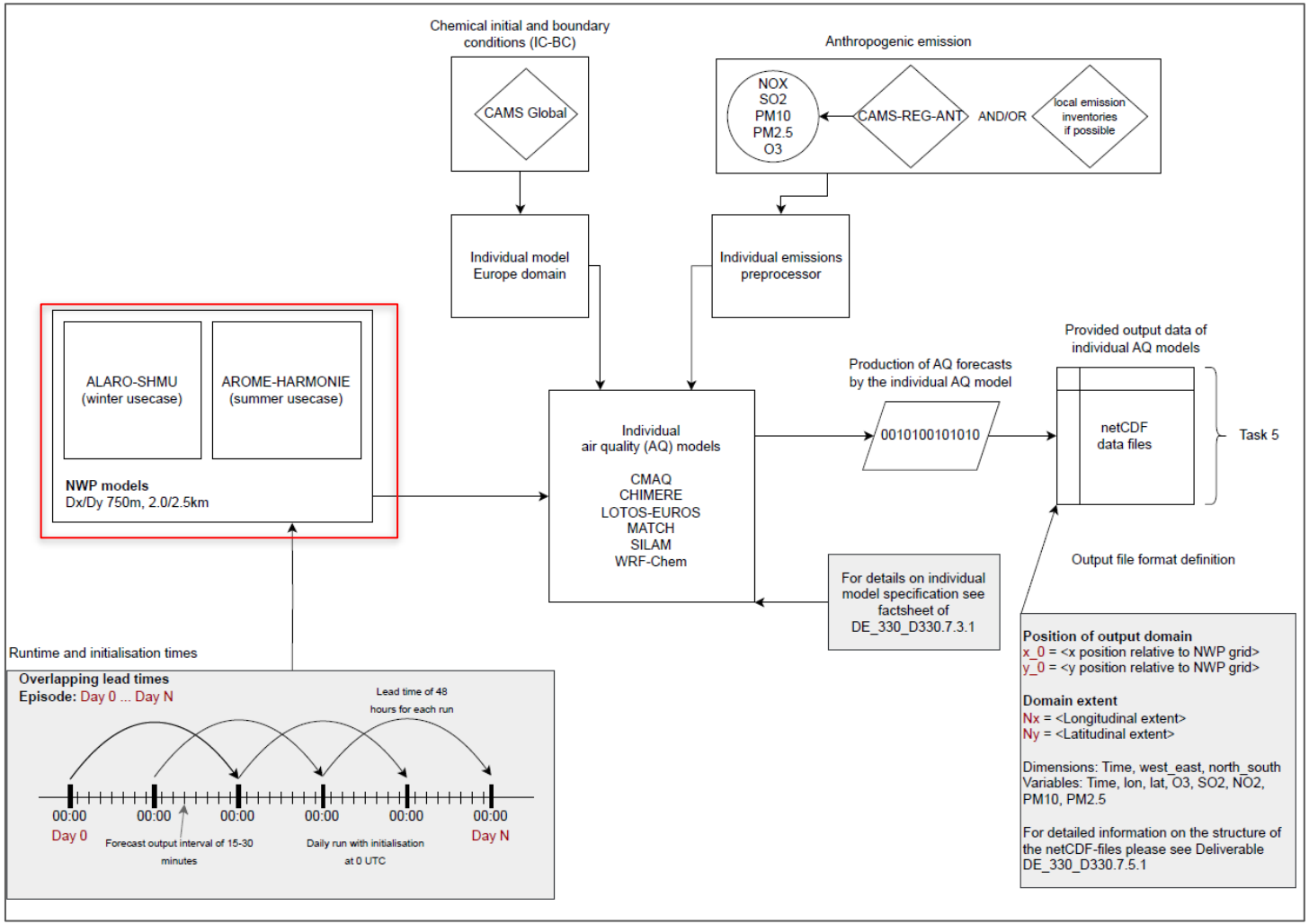
- The **modelling groups will adapt and develop their run scripts and environments** in a way that it is possible to set up model runs (domains, grid etc.) and to start the whole modelling chain from pre- to post-processing via a harmonised input file. The format and content of this file will be defined in this task.

- The models WRF-Chem and CMAQ will be set up to run next to the On-Demand Extremes hyper resolution NWP model on the same platform. The models will be implemented with a horizontal resolution of 750 m.

- The **quasi-operational environments will be used to run the models for the selected use cases** which will be simulated in this task by all modelling groups. All model outputs will be prepared in a pre-defined data format and further used to evaluate the model performance.

- The **concept of how end-users could use the tailored products of the on-demand AQ-impact model** in future phases of DestinE is that they will have flexibility, e.g. the freedom to set up their own modelling domains.


Chemical initial and boundary conditions (IC-BC)
CAMS Global
Anthropogenic emission
NOX
SO2
PM10
PM2.5
O3
CAMS-REG-ANT
AND/OR
local emission inventories if possible
Individual model Europe domain
Individual emissions preprocessor
ALARO-SHMU (winter usecase)
AROME-HARMONIE (summer usecase)
NWP models
Dx/Dy 750m, 2.0/2.5km
Individual air quality (AQ) models
CMAQ
CHIMERE
LOTOS-EUROS
MATCH
SILAM
WRF-Chem
Production of AQ forecasts by the individual AQ model
0010100101010
Provided output data of individual AQ models
netCDF data files
Task 5
For details on individual model specification see factsheet of DE_330_D330.7.3.1
Output file format definition
Position of output domain
x_0 = <x position relative to NWP grid>
y_0 = <y position relative to NWP grid>
Domain extent
Nx = <Longitudinal extent>
Ny = <Latitudinal extent>
Dimensions: Time, west_east, north_south
Variables: Time, lon, lat, O3, SO2, NO2, PM10, PM2.5
For detailed information on the structure of the netCDF-files please see Deliverable DE_330_D330.7.5.1
Runtime and initialisation times
Overlapping lead times
Episode: Day 0 ... Day N
Lead time of 48 hours for each run
00:00
Day 0
00:00
00:00
00:00
00:00
00:00
Day N
Forecast output interval of 15-30 minutes
Daily run with initialisation at 0 UTC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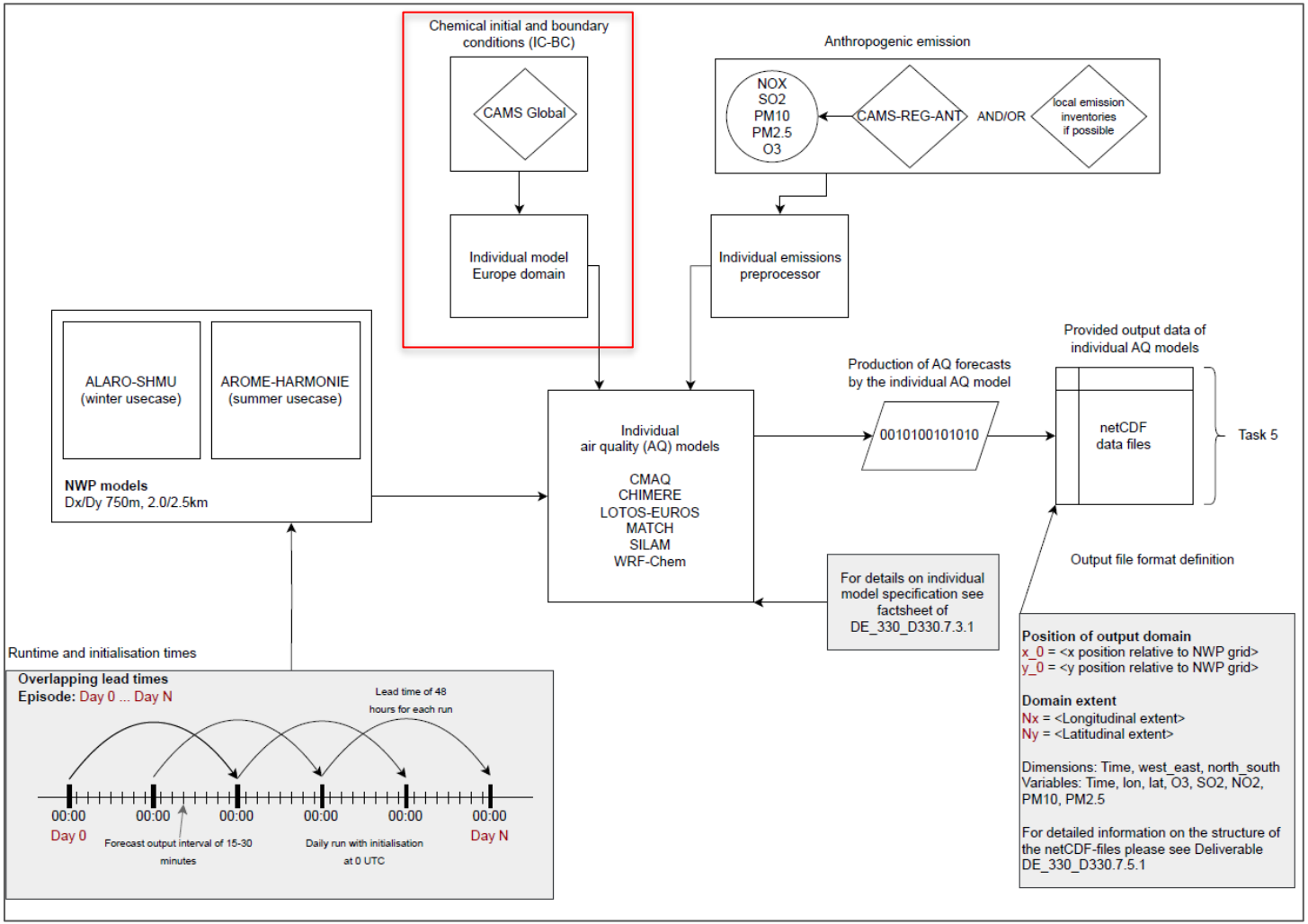
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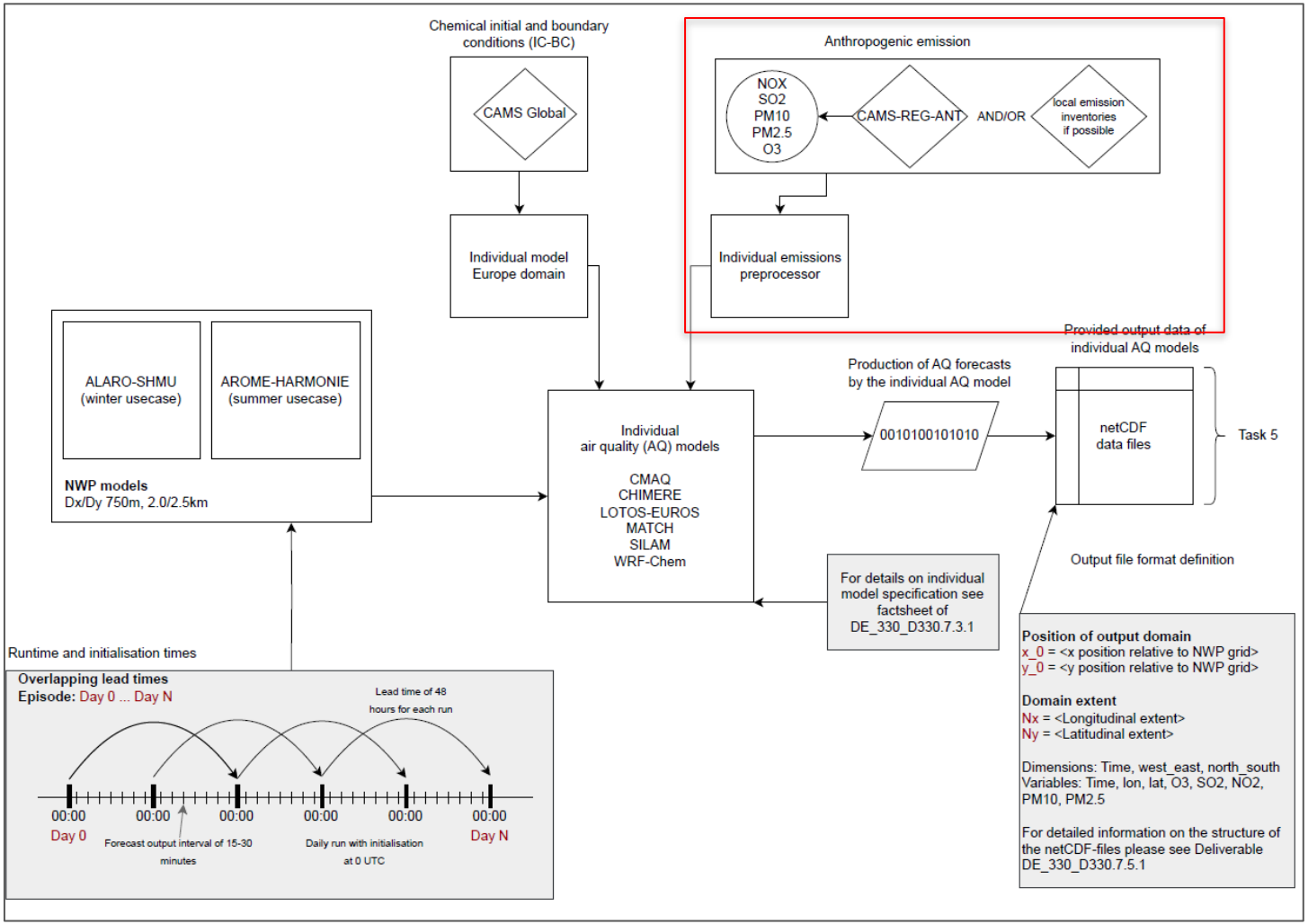
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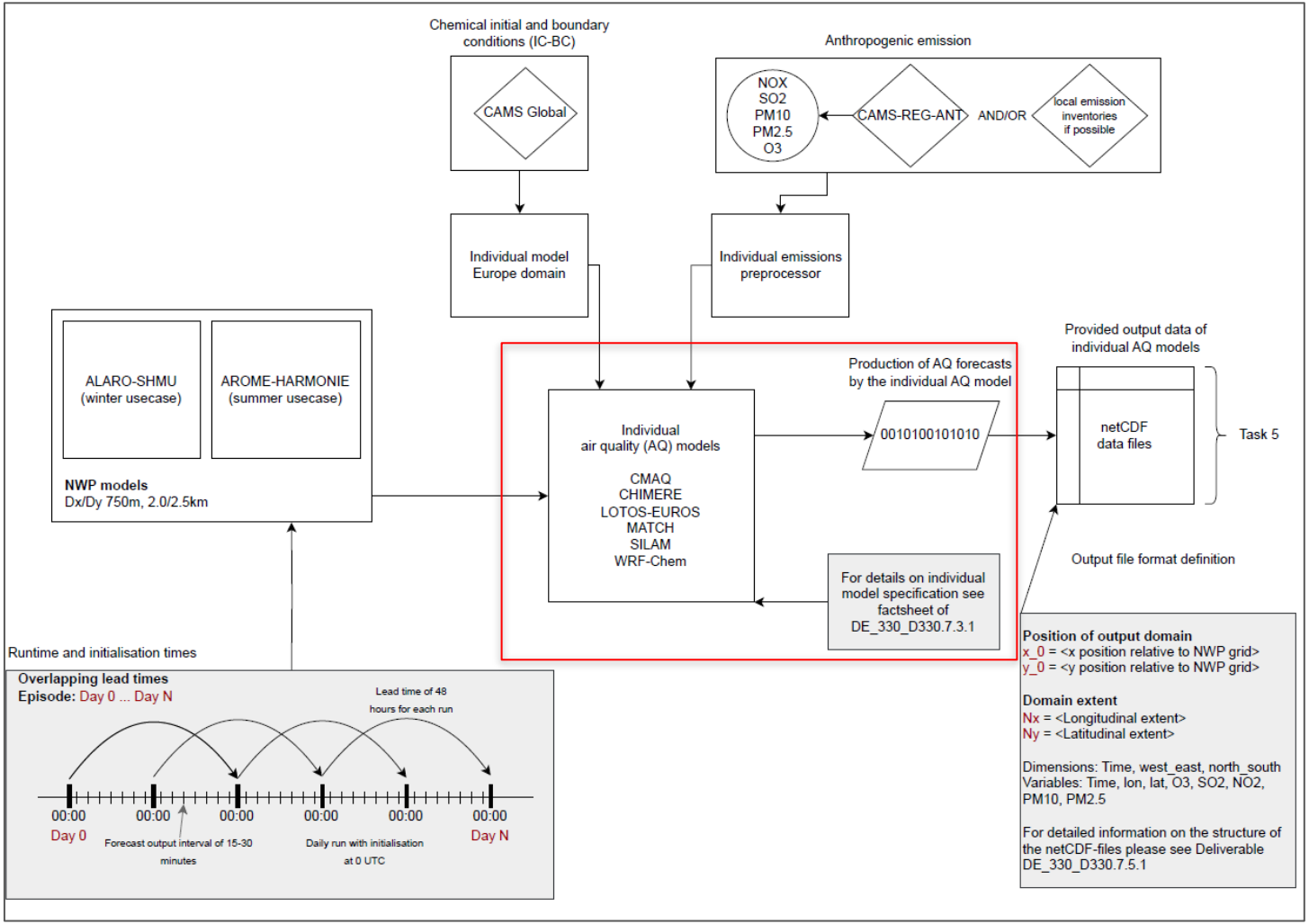
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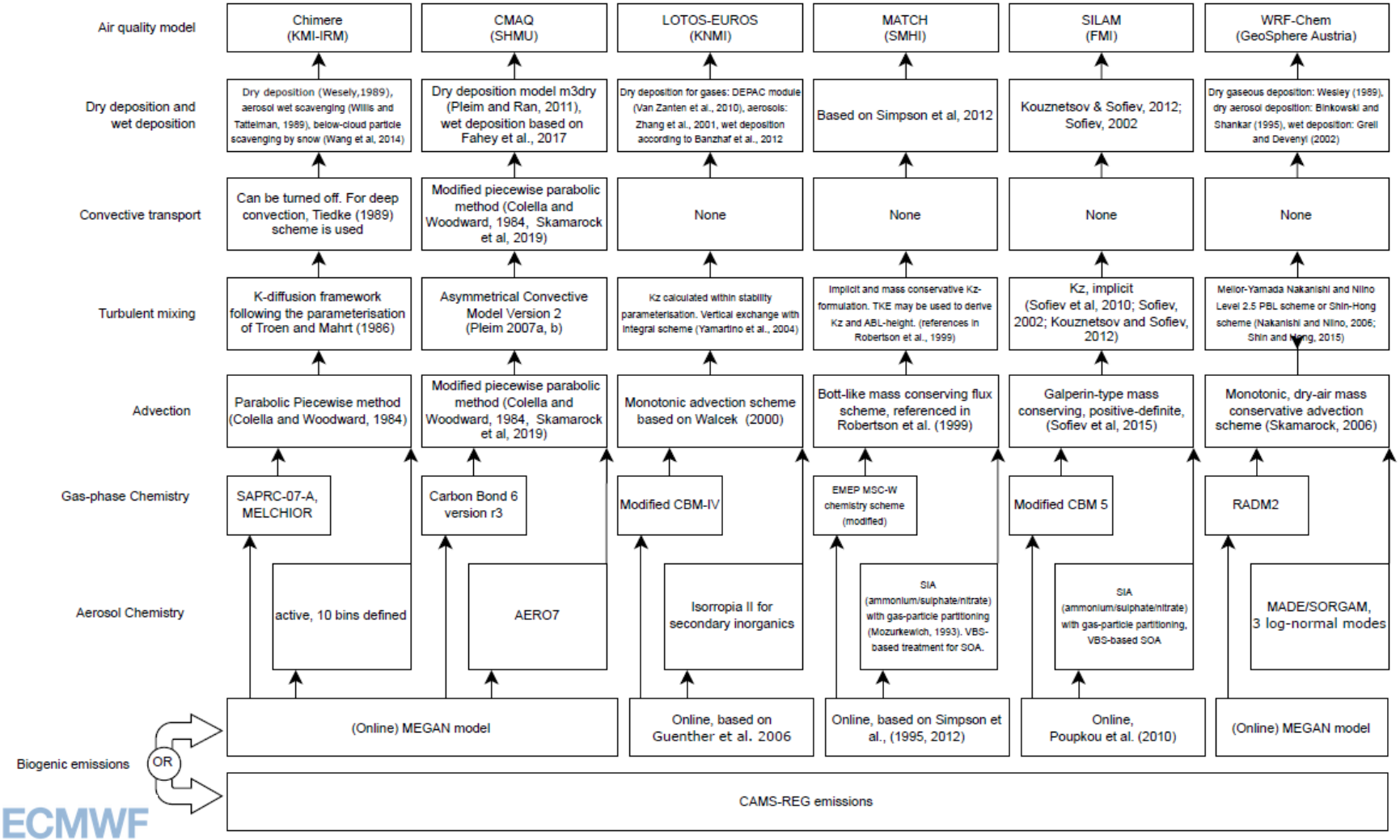
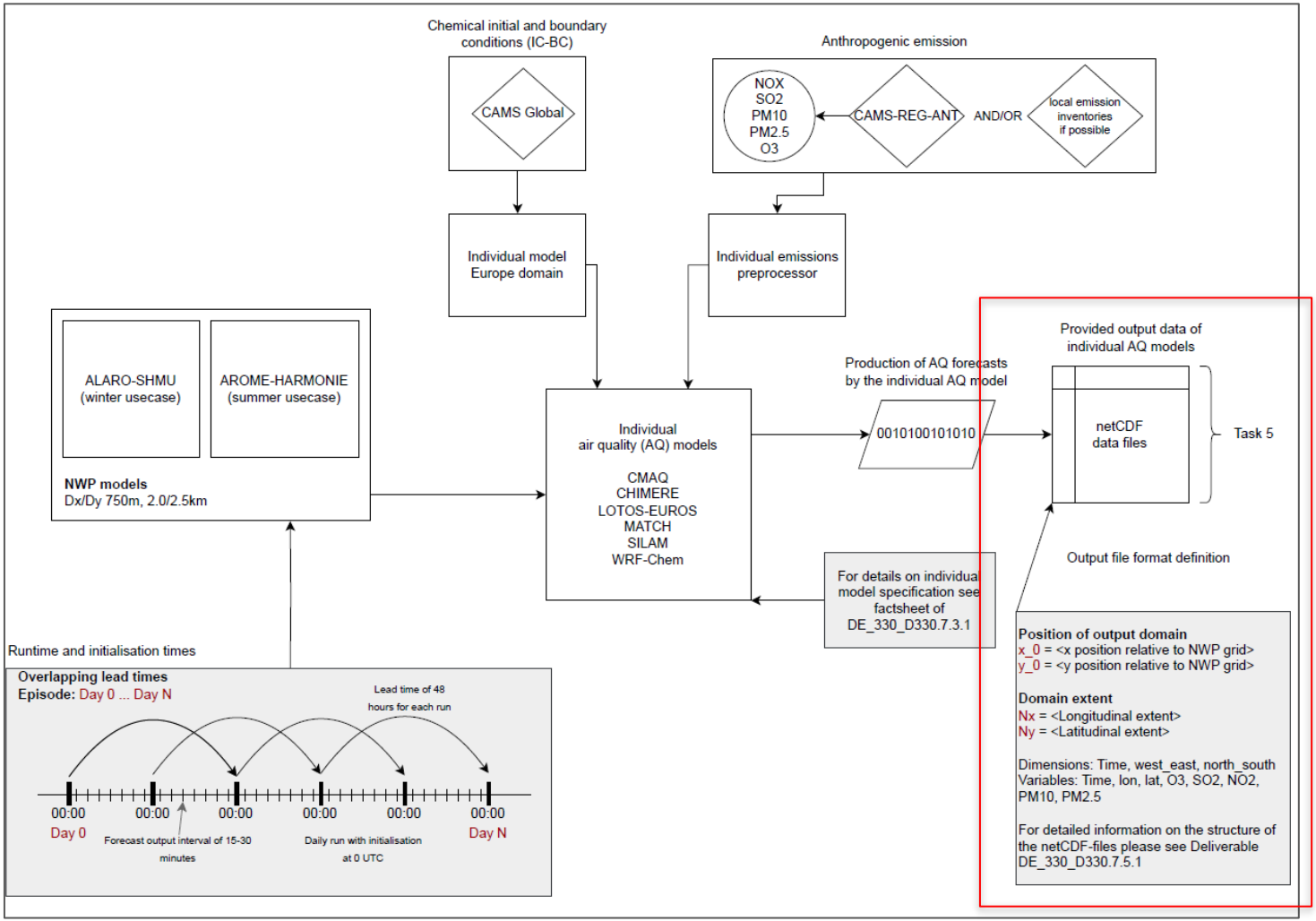

Air quality model
Chimere (KMI-IRM)
CMAQ (SHMU)
LOTOS-EUROS (KNMI)
MATCH (SMHI)
SILAM (FMI)
WRF-Chem (GeoSphere Austria)
Dry deposition and wet deposition
Dry deposition (Wesely,1989), aerosol wet scavenging (Willis and Tattelman, 1989), below-cloud particle scavenging by snow (Wang et al, 2014)
Dry deposition model m3dry (Pleim and Ran, 2011), wet deposition based on Fahey et al., 2017
Dry deposition for gases: DEPAC module (Van Zanten et al., 2010), aerosols: Zhang et al., 2001, wet deposition according to Banzhaf et al., 2012
Based on Simpson et al, 2012
Kouznetsov & Sofiev, 2012; Sofiev, 2002
Dry gaseous deposition: Wesley (1989), dry aerosol deposition: Binkowski and Shankar (1995), wet deposition: Grell and Devenyi (2002)
Convective transport
Can be turned off. For deep convection, Tiedke (1989) scheme is used
Modified piecewise parabolic method (Colella and Woodward, 1984, Skamarock et al, 2019)
None
None
None
None
Turbulent mixing
K-diffusion framework following the parameterisation of Troen and Mahrt (1986)
Asymmetrical Convective Model Version 2 (Pleim 2007a, b)
Kz calculated within stability parameterisation. Vertical exchange with integral scheme (Yamartino et al., 2004)
Implicit and mass conservative Kz-formulation. TKE may be used to derive Kz and ABL-height. (references in Robertson et al., 1999)
Kz, implicit (Sofiev et al, 2010; Sofiev, 2002; Kouznetsov and Sofiev, 2012)
Mellor-Yamada Nakanishi and Niino Level 2.5 PBL scheme or Shin-Hong scheme (Nakanishi and Niino, 2006; Shin and Hong, 2015)
Advection
Parabolic Piecewise method (Colella and Woodward, 1984)
Modified piecewise parabolic method (Colella and Woodward, 1984, Skamarock et al, 2019)
Monotonic advection scheme based on Walcek (2000)
Bott-like mass conserving flux scheme, referenced in Robertson et al. (1999)
Galperin-type mass conserving, positive-definite, (Sofiev et al, 2015)
Monotonic, dry-air mass conservative advection scheme (Skamarock, 2006)
Gas-phase Chemistry
SAPRC-07-A, MELCHIOR
Carbon Bond 6 version r3
Modified CBM-IV
EMEP MSC-W chemistry scheme (modified)
Modified CBM 5
RADM2
Aerosol Chemistry
active, 10 bins defined
AERO7
Isorropia II for secondary inorganics
SIA (ammonium/sulphate/nitrate) with gas-particle partitioning (Mozurkewich, 1993). VBS-based treatment for SOA.
SIA (ammonium/sulphate/nitrate) with gas-particle partitioning, VBS-based SOA
MADE/SORGAM, 3 log-normal modes
Biogenic emissions
OR
(Online) MEGAN model
Online, based on Guenther et al. 2006
Online, based on Simpson et al., (1995, 2012)
Online, Poupkou et al. (2010)
(Online) MEGAN model
CAMS-REG emissions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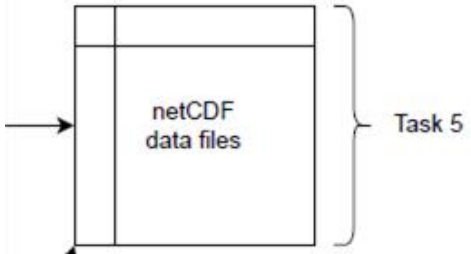


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Dimensions: Time, west_east, north_south
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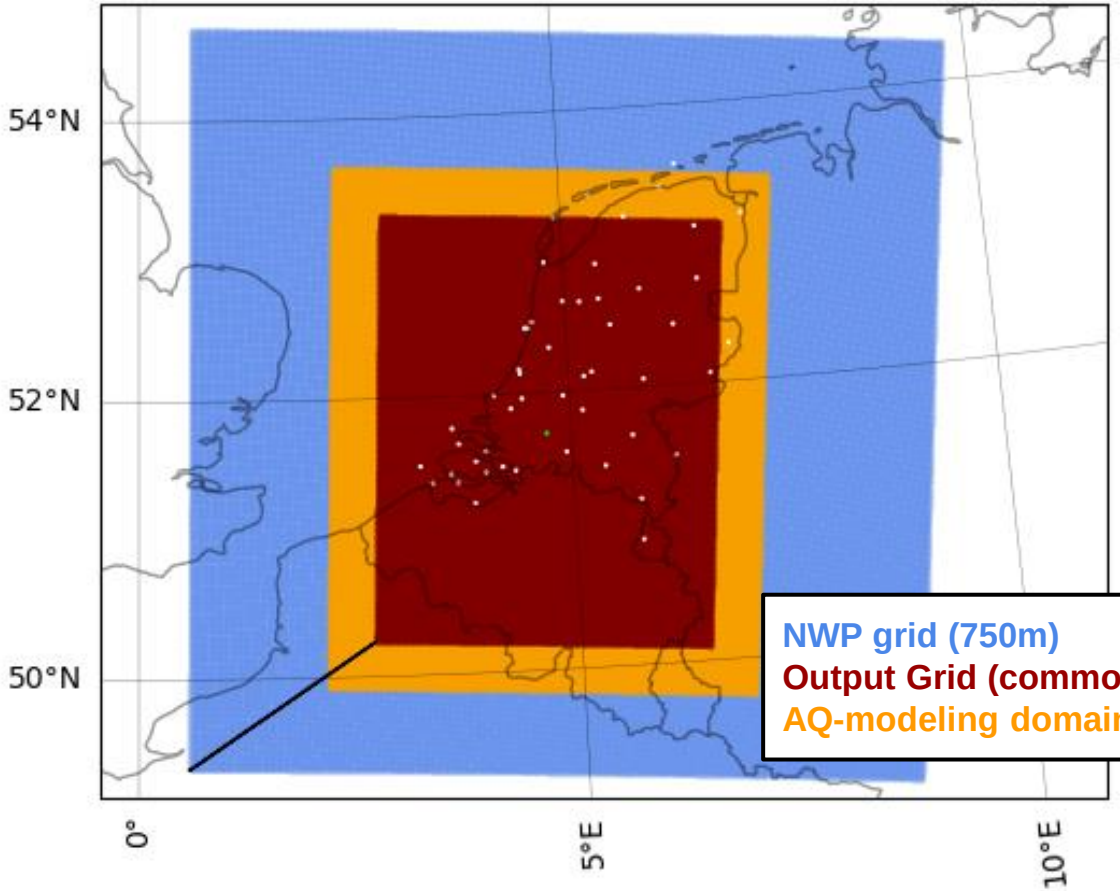
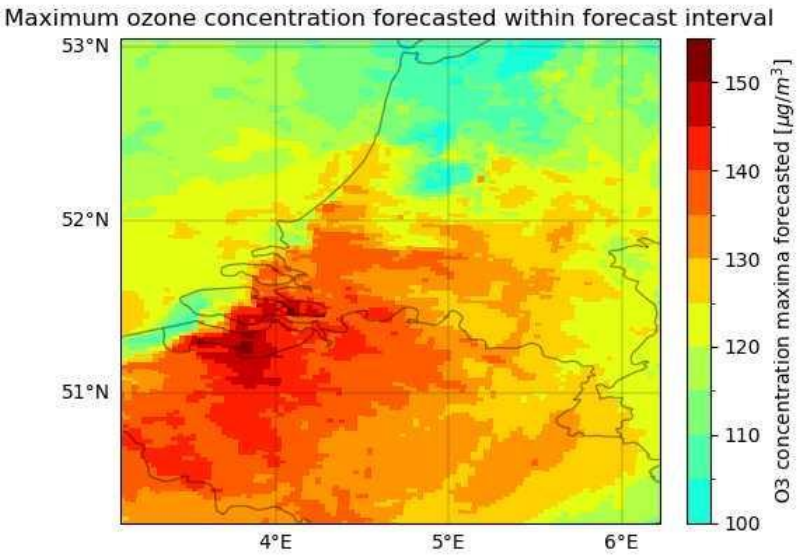
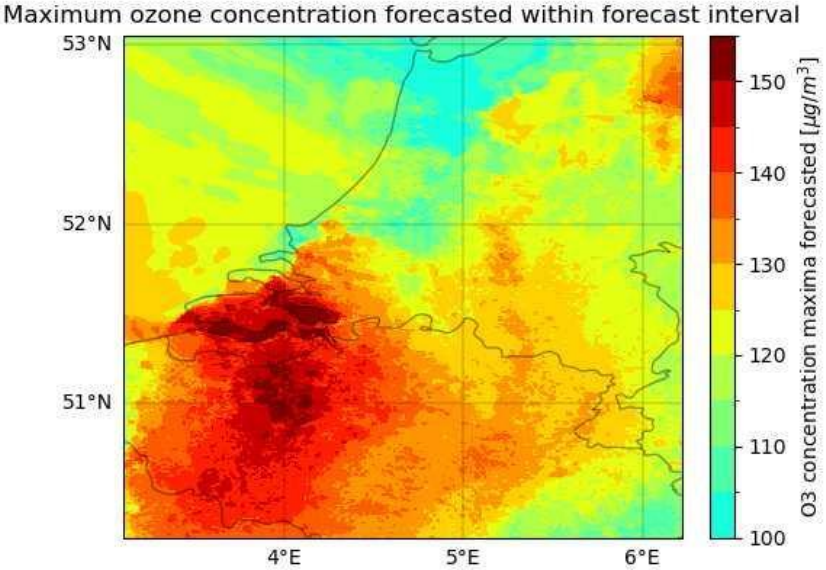


# Summer case - preliminary results

## Modelled ozone maximum concentrations for different resolutions



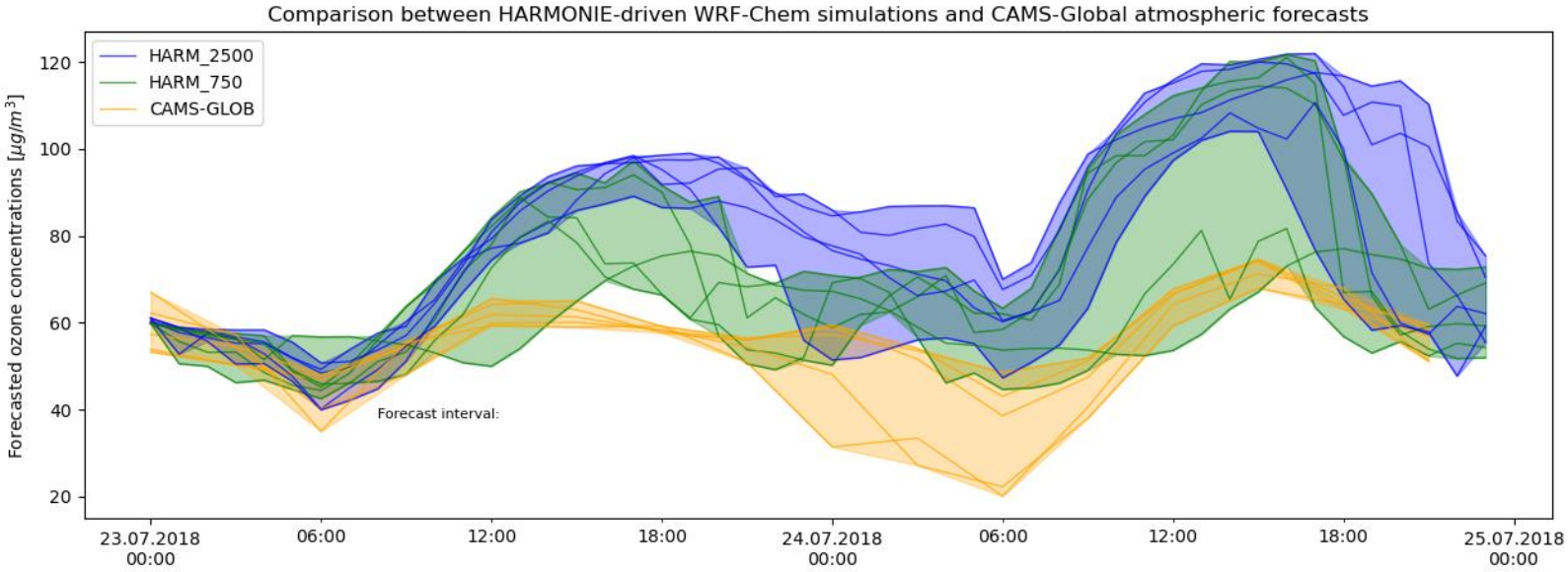

WRF-Chem model setting: HARMONIE-2500m
Forecast interval: 23.07.18 00:00 - 27.07.18 23:00




WRF-Chem model setting: HARMONIE-750m
Forecast interval: 23.07.18 00:00 - 27.07.18 23:00

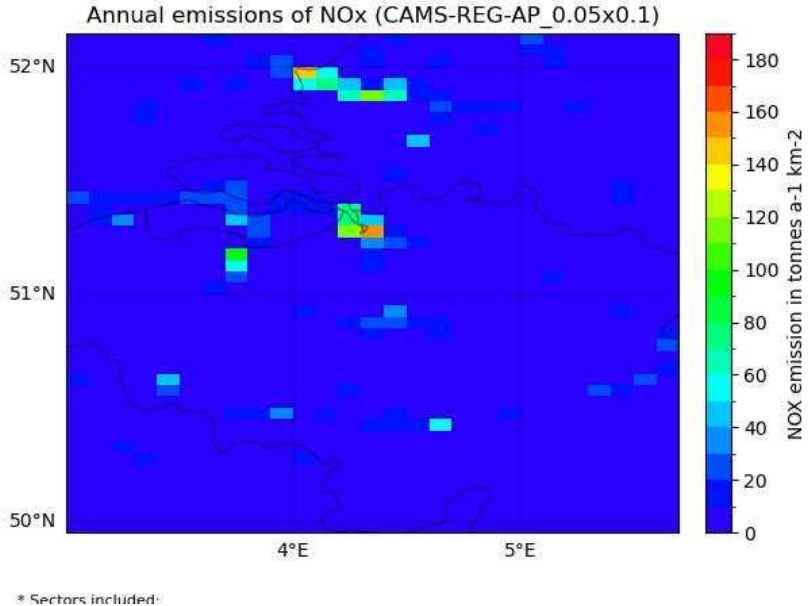
# Summer case - preliminary results

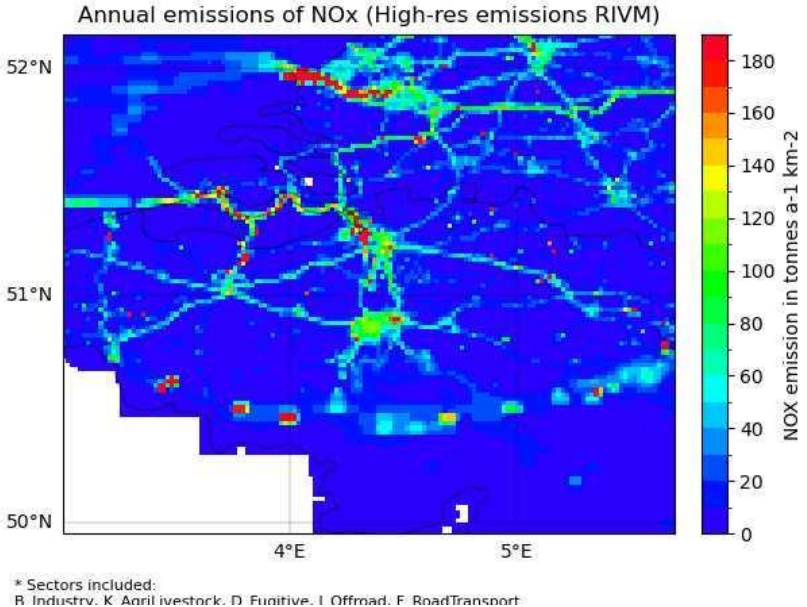
## Modelled ozone concentrations for selected urban stations



# Summer case - preliminary results

## Emissions



# Upcoming

- **Analysis of the use cases**
  - Final adjustments to the NWP-AQ interface
  - Ensemble
  - Evaluation
- **Phase II**
  - Tasks:
    - Emission preparation
    - Further model development toward sub km applications
    - (Quasi-)Operationalisation
    - Triggering
    - Output preparation / dissemination / end user needs
    - Evaluation


Tasks

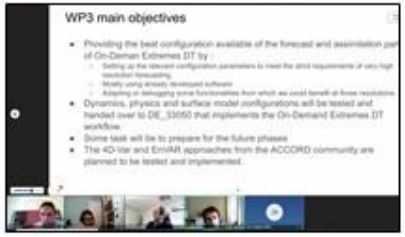

Consequences of a 20 month project period


DE_33051: workflow management and scripting


WP2 Code adaptation to CPUs and accelerators


DE_33060: Main objectives

# Thank you!


WP3 main objectives


DE_33070 Impact modelling – Air Quality


Open questions suggested for the discussions in the pre-KO meeting


IPR & licensing in the context of DestinE/DE_330
Pre-KO meeting 5-6 Sept 2022
Claudia Vacher


DE_33080: Impact modelling – Renewable energy